Appendix A: spherical droplet parallel to the slow motion of the plate

A.1 Introduction

The motion of droplets of one fluid dispersed in a second, immiscible fluid plays an important role in a variety of natural and industrial processes, such as raindrop formation, the mechanics and rheology of emulsions, liquid-liquid extraction, and sedimentation phenomena. The creeping-flow translation of a single spherical droplet of radius a in an unbounded medium of viscosity η was first analyzed independently by Hadamard (1911) and Rybczynski (1911). Assuming continuous velocity and continuous tangential shearing stress across the interface between the fluid phases in the absence of surface active agents, they found that the force exerted on the fluid sphere by the surrounding fluid is

$$\mathrm{F}_0 = -6\pi\eta a \frac{3\eta^* + 2}{3\eta^* + 3} \mathrm{U} \,. \qquad [A1]$$

Here, U is the migration velocity of the droplet and η^* is the internal-to-external viscosity ratio. Since the fluid properties are arbitrary, Eq. [A1] degenerates to the case of motion of a solid sphere (Stokes' law) when the viscosity of the droplet becomes infinite and to the case of motion of a gas bubble when the viscosity approaches zero.

During the translation of a fluid sphere in a second, immiscible fluid, the interfacial stresses acting at the droplet surface tend to deform it. If the motion is sufficiently slow or the droplet is sufficiently small, the droplet will in the first approximation be spherical. The problems associated with the shape of a droplet undergoing distortion, when inertial effects are no longer negligible, were discussed in the literature (Taylor and Acrivos, 1964; Dandy and Leal, 1989).

In many practical applications of low-Reynolds-number motion, droplets are not isolated and the surrounding fluid is externally bounded by solid walls. Thus, it is important to determine if the presence of neighboring boundaries significantly affects the movement of a droplet. Using spherical bipolar coordinates, Bart (1968) and Rushton and Davies (1973) examined the motion of a spherical droplet settling normal to a plane interface between two immiscible viscous fluids. This work is an extension of the analyses of Maude (1961) and Brenner (1961), who independently analyzed the fluid motion generated by a rigid sphere moving perpendicular to a solid plane surface or to a free surface plane. Wacholder and Weihs (1972) also utilized bipolar coordinates to study the motion of a fluid sphere through another fluid normal to a rigid or free plane surface; their calculations agree with the results obtained by Bart (1968) in these limits. Hetsroni et al. (1970) used a method of reflections to solve for the terminal settling velocity of a spherical droplet moving axially at an arbitrary radial location within a long circular tube filled with a viscous fluid. The wall effects experienced by a fluid sphere moving along the axis of a circular tube were also examined by using the reciprocal theorem (Brenner, 1971) and an approximative approach (Coutanceau and Thizon, 1981).

The parallel motion of a droplet in a quiescent fluid at any position between two parallel flat plates was studied by Shapira and Haber (1988) using the method of reflections. Approximate solutions for the hydrodynamic drag force exerted on the droplet were obtained to the first order of $a/(b+c)$, where b and c are the respective distances from the droplet center to the two plates. Obviously, this result can not be sufficiently accurate when the value of $a/(b+c)$ is large, say, >0.2. The purpose of this appendix is to obtain an exact solution for the slow motion of a spherical droplet parallel to two plane walls at an arbitrary position between them. The creeping-flow equations applicable to the system are solved by using a combined analytical-numerical method with a boundary collocation technique (Ganatos *et al*., 1980), and the wall-corrected drag force acting on the droplet is obtained with good convergence for various cases. For the special case of movement of a droplet with infinite viscosity, our calculations show excellent agreement with the available solutions in the literature for the corresponding motion of a solid sphere.

A.2 Analysis

We consider the steady creeping motion caused by a spherical droplet of radius a translating with a constant velocity $\mathrm{U} = U\mathrm{e}_x$ in an immiscible fluid parallel to two infinite plane walls whose distances from the center of the droplet are b and c, as shown in Fig. A1. Here (x, y, z), (ρ, ϕ, z), and (r, θ, ϕ) denote the rectangular, circular cylindrical, and spherical coordinate systems, respectively, with the origin of coordinates at the droplet center, and $\mathbf{e}_x$ is the unit vector in the x direction. We set $b \le c$ throughout this work, without the loss of generality. The droplet is assumed to be sufficiently small so that interfacial tension (which is assumed to be fairly large) maintains its spherical shape. The fluid is at rest far away from the droplet. The objective is to determine the correction to Eq. [A1] for the motion of the droplet due to the presence of the plane walls.

The fluids inside and outside the droplet are assumed to be incompressible and Newtonian. Owing to the low Reynolds number, the fluid motion is governed by the Stokes equations,

$$\eta\nabla^2\mathrm{v} - \nabla p = 0\,, \qquad \nabla\cdot\mathrm{v} = 0 \qquad (r \ge a), \qquad \text{[A2a,b]}$$

$$\eta_1\nabla^2\mathrm{v}_1 - \nabla p_1 = 0\,, \qquad \nabla\cdot\mathrm{v}_1 = 0 \qquad (r \le a), \qquad \text{[A3a,b]}$$

where v_1 and v are the fluid velocity fields for the flow inside the droplet and for the external flow, respectively, p_1 and p are the corresponding dynamic pressure distributions, and η_1 is the viscosity of the droplet.

The boundary conditions for the fluid velocity at the droplet surface, on the plane walls, and far removed from the droplet are

$$r = a: \qquad \mathrm{e}_r\cdot(\mathrm{v} - U\mathrm{e}_x) = 0\,, \qquad \text{[A4a]}$$

$$\mathrm{v} = \mathrm{v}_1\,, \qquad \text{[A4b]}$$

$$(\mathrm{I} - \mathrm{e}_r\mathrm{e}_r)\mathrm{e}_r : (\tau - \tau_1) = 0\,, \qquad \text{[A4c]}$$

$$z = c\,, -b: \qquad \mathrm{v} = 0\,, \qquad \text{[A4d]}$$

$$\rho \to \infty: \qquad \mathrm{v} = 0\,. \qquad \text{[A4e]}$$

Here, $\boldsymbol{\tau} = \eta[\nabla\mathrm{v} + (\nabla\mathrm{v})^T]$ and $\boldsymbol{\tau}_1 = \eta_1[\nabla\mathrm{v}_1 + (\nabla\mathrm{v}_1)^T]$ are viscous stress tensors for the external flow and the flow inside the droplet, respectively; $\mathbf{e}_r$ together with $\mathbf{e}_\theta$ and $\mathbf{e}_\phi$ are the unit vectors in spherical coordinates; $\mathbf{I}$ is the unit dyadic.

In view of the linearity of the governing equations and boundary conditions, the external velocity field $\mathbf{v}$ can be decomposed into two contributions (Ganatos *et al.*, 1980),

$$\mathbf{v} = \mathbf{v}_w + \mathbf{v}_s . \qquad \text{[A5]}$$

Here, $\mathbf{v}_w$ is a solution of Eq. [A2] in rectangular coordinates that represents the disturbance produced by the plane walls and is given by

$$\mathbf{v}_w = v_{wx}\mathbf{e}_x + v_{wy}\mathbf{e}_y + v_{wz}\mathbf{e}_z , \qquad \text{[A6]}$$

where $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$ are the unit vectors in rectangular coordinates, and v_{wx}, v_{wy}, v_{wz} are the double Fourier integrals,

$$v_{wx} = \int_0^\infty \int_0^\infty D_1(\alpha,\beta,z)\cos(\alpha x)\cos(\beta y)d\alpha\, d\beta , \qquad \text{[A7a]}$$

$$v_{wy} = \int_0^\infty \int_0^\infty D_2(\alpha,\beta,z)\sin(\alpha x)\sin(\beta y)d\alpha\, d\beta , \qquad \text{[A7b]}$$

$$v_{wz} = \int_0^\infty \int_0^\infty D_3(\alpha,\beta,z)\sin(\alpha x)\cos(\beta y)d\alpha\, d\beta . \qquad \text{[A7c]}$$

In Eq. [A7],

$$D_1 = [X^*(1+\frac{\alpha^2}{\kappa}z) - X^{**}\frac{\alpha\beta}{\kappa}z - X^{***}\alpha z]e^{\kappa z}$$
$$+[Y^*(1-\frac{\alpha^2}{\kappa}z) + Y^{**}\frac{\alpha\beta}{\kappa}z - Y^{***}\alpha z]e^{-\kappa z} , \qquad \text{[A8a]}$$

$$D_2 = [-X^*\frac{\alpha\beta}{\kappa}z + X^{**}(1+\frac{\beta^2}{\kappa}z) + X^{***}\beta z]e^{\kappa z}$$
$$+[Y^*\frac{\alpha\beta}{\kappa}z + Y^{**}(1-\frac{\beta^2}{\kappa}z) + Y^{***}\beta z]e^{-\kappa z} , \qquad \text{[A8b]}$$

$$D_3 = [X^*\alpha z - X^{**}\beta z + X^{***}(1-\kappa z)]e^{\kappa z}$$

$$+[Y^*\alpha z - Y^{**}\beta z + Y^{***}(1+\kappa z)]e^{-\kappa z} , \qquad \text{[A8c]}$$

where the starred X and Y are unknown functions of separation variables α and β, and $\kappa^2 = \alpha^2 + \beta^2$.

The second part of $\mathbf{v}$ in Eq. [A5], denoted by $\mathbf{v}_s$, is a solution of Eq. [A2] in spherical coordinates representing the disturbance generated by the droplet and is given by

$$\mathbf{v}_s = v_{sx}\mathbf{e}_x + v_{sy}\mathbf{e}_y + v_{sz}\mathbf{e}_z \,, \qquad \text{[A9]}$$

where

$$v_{sx} = \sum_{n=1}^{\infty}(A_n A'_n + B_n B'_n + C_n C'_n), \qquad \text{[A10a]}$$

$$v_{sy} = \sum_{n=1}^{\infty}(A_n A''_n + B_n B''_n + C_n C''_n), \qquad \text{[A10b]}$$

$$v_{sz} = \sum_{n=1}^{\infty}(A_n A'''_n + B_n B'''_n + C_n C'''_n). \qquad \text{[A10c]}$$

In Eq. [A10], the primed A_n, B_n, and C_n are functions of position involving associated Legendre functions of $\cos\theta$ defined in the appendix, which were also given by Eq. [2.6] of Ganatos *et al*. (1980), and A_n, B_n, and C_n are unknown constants. Note that the boundary condition in Eq. [A4e] is immediately satisfied by a solution of the form given by Eqs. [A5]-[A10].

The solution to Eq. [A3] for the internal velocity field can be expressed as

$$\mathrm{v}_1 = v_{1r}\mathrm{e}_r + v_{1\theta}\mathrm{e}_\theta + v_{1\phi}\mathrm{e}_\phi \,, \qquad \text{[A11]}$$

where

$$v_{1r} = \sum_{n=1}^{\infty} n P_n^1(\mu)(\overline{C}_n\, r^{n-1} + \overline{A}_n\, r^{n+1})\cos\phi \,, \qquad \text{[A12a]}$$

$$v_{1\theta} = \sum_{n=1}^{\infty}[\overline{B}_n\, r^n P_n^1(\mu)(1-\mu^2)^{-1/2} - (1-\mu^2)^{1/2}\frac{dP_n^1(\mu)}{d\mu}(\overline{C}_n\, r^{n-1} - \overline{A}_n \frac{n+3}{n+1} r^{n+1})]\cos\phi \,, \qquad \text{[A12b]}$$

$$v_{1\phi} = \sum_{n=1}^{\infty}[\overline{B}_n\, r^n (1-\mu^2)^{1/2}\frac{dP_n^1(\mu)}{d\mu} - (1-\mu^2)^{-1/2} P_n^1(\mu)(\overline{C}_n\, r^{n-1} - \overline{A}_n \frac{n+3}{n+1} r^{n+1})]\sin\phi \,, \qquad \text{[A12c]}$$

P_n^m is the associated Legendre function of order *n* and degree *m*, μ is uesd to denote $\cos\theta$ for brevity, and $\overline{A}_n$, $\overline{B}_n$, and $\overline{C}_n$ are unknown constants. A solution of this form satisfies the requirement that the velocity is finite for any position within the droplet. Note that the solution for $\mathbf{v}_1$ contains only terms of $\cos\phi$ and $\sin\phi$ (and not higher-order harmonics) due to the symmetry of the geometry of the system.

A brief conceptual description of the solution procedure to determine the starred X and Y functions in Eq. [A8] and the constants A_n, B_n, C_n, $\overline{A}_n$, $\overline{B}_n$, and $\overline{C}_n$ in Eqs. [A10] and [A12] is given below to help follow the mathematical development. At first, boundary conditions (given by Eq. [A4d]) are exactly satisfied on the plane walls by using the Fourier transforms. This permits the unknown starred X and Y functions to be determined in terms of the coefficients A_n, B_n, and C_n. Then, the boundary conditions in Eqs. [A4a-c] on the surface of the droplet can be satisfied by making use of the collocation method, and the solution of the collocation matrix provides numerical values for the coefficients A_n, B_n, C_n, $\overline{A}_n$, $\overline{B}_n$, and $\overline{C}_n$.

Substitution of the velocity distribution $\mathbf{v}$ given by Eqs. [A5]-[A10] into the boundary conditions of Eq. [A4d] and application of the Fourier sine and cosine inversions on the variables x and y, respectively, lead to a solution for the functions D_1, D_2, and D_3 (or starred X and Y functions) in terms of the coefficients A_n, B_n, and C_n. After the substitution of this solution back into Eq. [A7] and utilization of the integral representations of the modified Bessel functions of the second kind, the external fluid velocity field can be expressed as

$$\mathrm{v} = v_x \mathrm{e}_x + v_y \mathrm{e}_y + v_z \mathrm{e}_z , \qquad \text{[A13]}$$

where

$$v_x = \sum_{n=1}^{\infty} [A_n (A'_n + \alpha'_n) + B_n (B'_n + \beta'_n) + C_n (C'_n + \gamma'_n)] , \qquad \text{[A14a]}$$

$$v_y = \sum_{n=1}^{\infty} [A_n (A''_n + \alpha''_n) + B_n (B''_n + \beta''_n) + C_n (C''_n + \gamma''_n)] , \qquad \text{[A14b]}$$

$$v_z = \sum_{n=1}^{\infty} [A_n (A'''_n + \alpha'''_n) + B_n (B'''_n + \beta'''_n) + C_n (C'''_n + \gamma'''_n)] . \qquad \text{[A14c]}$$

Here, the primed α_n, β_n, and γ_n are complicated functions of position in the form of integration (which must be performed numerically) defined by Eq. [C1] of Ganatos *et al*. (1980).

The boundary conditions that remain to be satisfied are those on the droplet surface. Substituting Eqs. [A11]-[A14] into Eqs. [A4a-c], one obtains

$$\sum_{n=1}^{\infty} [A_n A_n^*(a,\mu,\phi) + B_n B_n^*(a,\mu,\phi) + C_n C_n^*(a,\mu,\phi)] = U_x (1-\mu^2)^{1/2} \cos\phi , \qquad \text{[A15a]}$$

$$\sum_{n=1}^{\infty}[A_n A_n^*(a,\mu,\phi)+B_n B_n^*(a,\mu,\phi)+C_n C_n^*(a,\mu,\phi)]-\sum_{n=1}^{\infty}[\overline{C}_n\ na^{n-1}P_n^1(\mu)$$

$$+\overline{A}_n\ na^{n+1}P_n^1(\mu)]\cos\phi=0\,, \qquad \text{[A15b]}$$

$$\sum_{n=1}^{\infty}[A_n A_n^{**}(a,\mu,\phi)+B_n B_n^{**}(a,\mu,\phi)+C_n C_n^{**}(a,\mu,\phi)]$$

$$-\sum_{n=1}^{\infty}[\overline{B}_n\ a^n(1-\mu^2)^{-1/2}P_n^1(\mu)-\overline{C}_n\ a^{n-1}(1-\mu^2)^{1/2}\frac{dP_n^1}{d\mu}$$

$$-\overline{A}_n\frac{n+3}{n+1}a^{n+1}(1-\mu^2)^{1/2}\frac{dP_n^1}{d\mu}]\cos\phi=0\,, \qquad \text{[A15c]}$$

$$\sum_{n=1}^{\infty}[A_n A_n^{***}(a,\mu,\phi)+B_n B_n{}^{***}(a,\mu,\phi)+C_n C_n{}^{***}(a,\mu,\phi)]$$

$$-\sum_{n=1}^{\infty}[\overline{B}_n\ a^n(1-\mu^2)^{1/2}\frac{dP_n^1(\mu)}{d\mu}-\overline{C}_n\ a^{n-1}(1-\mu^2)^{-1/2}P_n^1(\mu)\,,$$

$$-\overline{A}_n\frac{n+3}{n+1}a^{n+1}(1-\mu^2)^{-1/2}P_n^1(\mu)]\sin\phi=0 \qquad \text{[A15d]}$$

$$\sum_{n=1}^{\infty}\{(\frac{\partial}{\partial r}-\frac{1}{r})[A_n A_n^{**}(r,\mu,\phi)+B_n B_n^{**}(r,\mu,\phi)+C_n C_n^{**}(r,\mu,\phi)]$$

$$-\frac{(1-\mu^2)^{1/2}}{r}\frac{\partial}{\partial\mu}[A_n A_n^*(r,\mu,\phi)+B_n B_n^*(r,\mu,\phi)+C_n C_n^*(r,\mu,\phi)]\}_{r=a}$$

$$-\eta^*\sum_{n=1}^{\infty}[\overline{B}_n(n-1)a^{n-1}P_n^1(\mu)(1-\mu^2)^{-1/2}$$

$$-\overline{C}_n 2(n-1)a^{n-2}(1-\mu^2)^{1/2}\frac{dP_n^1(\mu)}{d\mu}$$

$$-\overline{A}_n\frac{n(n+2)}{n+1}a^n(1-\mu^2)^{1/2}\frac{dP_n^1(\mu)}{d\mu}]\cos\phi=0\,, \qquad \text{[A15e]}$$

$$\sum_{n=1}^{\infty}\{(\frac{\partial}{\partial r}-\frac{1}{r})[A_n A_n^{***}(r,\mu,\phi)+B_n B_n^{***}(r,\mu,\phi)+C_n C_n^{***}(r,\mu,\phi)]$$

$$+\frac{(1-\mu^2)^{-1/2}}{r}\frac{\partial}{\partial\phi}[A_n A_n^*(r,\mu,\phi)+B_n B_n^*(r,\mu,\phi)+C_n C_n^*(r,\mu,\phi)]\}_{r=a}$$

$$-\eta^*\sum_{n=1}^{\infty}[\overline{B}_n(n-1)a^{n-1}(1-\mu^2)^{1/2}\frac{dP_n^1(\mu)}{d\mu}-\overline{C}_n 2(n-1)a^{n-2}(1-\mu^2)^{-1/2}P_n^1(\mu)$$

$$-\overline{A}_n\frac{n(n+2)}{n+1}a^n(1-\mu^2)^{-1/2}P_n^1(\mu)]\sin\phi=0\,, \qquad \text{[A15f]}$$

where $\eta^*=\eta_1/\eta$. The starred A_n, B_n, and C_n functions in Eq. [A15] are defined by

$$A_n^*(r,\mu,\phi)=(1-\mu^2)^{1/2}(A_n'+\alpha_n')\cos\phi+(1-\mu^2)^{1/2}(A_n''+\alpha_n'')\sin\phi+\mu(A_n'''+\alpha_n'''),$$

[A16a]

$$B_n^*(r,\mu,\phi)=(1-\mu^2)^{1/2}(B_n'+\beta_n')\cos\phi+(1-\mu^2)^{1/2}(B_n''+\beta_n'')\sin\phi+\mu(B_n'''+\beta_n'''),$$

[A16b]

$$C_n^{*}(r,\mu,\phi) = (1-\mu^2)^{1/2}(C_n' + \gamma_n')\cos\phi + (1-\mu^2)^{1/2}(C_n'' + \gamma_n'')\sin\phi + \mu(C_n''' + \gamma_n''') \, ,$$

[A16c]

$$A_n^{**}(r,\mu,\phi) = \mu(A_n' + \alpha_n')\cos\phi + \mu(A_n'' + \alpha_n'')\sin\phi - (1-\mu^2)^{1/2}(A_n''' + \alpha_n''') \, ,$$

[A16d]

$$B_n^{**}(r,\mu,\phi) = \mu(B_n' + \beta_n')\cos\phi + \mu(B_n'' + \beta_n'')\sin\phi - (1-\mu^2)^{1/2}(B_n''' + \beta_n''') \, ,$$

[A16e]

$$C_n^{**}(r,\mu,\phi) = \mu(C_n' + \gamma_n')\cos\phi + \mu(C_n'' + \gamma_n'')\sin\phi - (1-\mu^2)^{1/2}(C_n''' + \gamma_n''') \, ,$$

[A16f]

$$A_n^{***}(r,\mu,\phi) = -(A_n' + \alpha_n')\sin\phi + (A_n'' + \alpha_n'')\cos\phi \, , \qquad \text{[A16g]}$$

$$B_n^{***}(r,\mu,\phi) = -(B_n' + \beta_n')\sin\phi + (B_n'' + \beta_n'')\cos\phi \, , \qquad \text{[A16h]}$$

$$C_n^{***}(r,\mu,\phi) = -(C_n' + \gamma_n')\sin\phi + (C_n'' + \gamma_n'')\cos\phi \, , \qquad \text{[A16i]}$$

where the primed A_n, B_n, C_n, α_n, β_n, and γ_n are functions of position in Eqs. [A10] and [A14].

Careful examination of Eq. [A15] shows that the solution of the coefficient matrix generated is independent of the ϕ coordinate of the boundary points on the spherical surface $r = a$. To satisfy the conditions in Eq. [A15] exactly along the entire surface of the droplet would require the solution of the entire infinite array of unknown constants A_n, B_n, C_n, $\overline{A}_n$, $\overline{B}_n$, and $\overline{C}_n$. However, the collocation technique (O'Brien, 1968; Ganatos *et al*., 1980; Keh and Tseng, 1992; Chen and Ye, 2000) enforces the boundary conditions at a finite number of discrete points on the half-circular generating arc of the droplet (from $\theta = 0$ to $\theta = \pi$) and truncates the infinite series in Eqs. [A12] and [A14] into finite ones. If the spherical boundary is approximated by satisfying the conditions of Eqs. [A4a-c] at N discrete points on its generating arc, the infinite series in Eqs. [A12] and [A14] are truncated after N terms, resulting in a system of 6N simultaneous linear algebraic equations in the truncated form of Eq.

[A15]. This matrix equation can be solved to yield the 6N unknown constants A_n, B_n, C_n, $\overline{A}_n$, $\overline{B}_n$, and $\overline{C}_n$ appearing in the truncated form of Eqs. [A12] and [A14]. The fluid velocity field is completely obtained once these coefficients are solved. Note that the definite integrals in Eq. [A15] after the substitution of Eq. [A16] must be performed numerically. The accuracy of the truncation technique can be improved to any degree by taking a sufficiently large value of N. Naturally, as $N \to \infty$ the truncation error vanishes and the overall accuracy of the solution depends only upon the numerical integration required in evaluating the matrix elements.

The drag force exerted by the external fluid on the spherical droplet can be determined from (Ganatos *et al*., 1980)

$$\mathrm{F} = -8\pi\eta\, A_1\, \mathrm{e}_x . \qquad \text{[A17]}$$

This expression shows that only the lowest-order coefficient A_1 contributes to the hydrodynamic force acting on the droplet.

A.3 Results and discussion

The solution for the slow motion of a spherical droplet parallel to two plane walls at an arbitrary position between them, obtained by using the boundary collocation technique described in the previous section, will be presented in this section. The system of linear algebraic equations to be solved for coefficients A_n, B_n, C_n, $\overline{A}_n$, $\overline{B}_n$, and $\overline{C}_n$ is constructed from Eq. [A15]. All the numerical intergrations to evaluate the starred A_n, B_n, and C_n functions (or the primed α_n, β_n, and γ_n functions) were done by the 40-point Gauss-Laguerre quadrature.

When specifying the points along the semicircular generating arc of the sphere where the boundary conditions are to be exactly satisfied, the first points that should be chosen are $\theta = 0$ and π, since these points define the projected area of the droplet normal to the direction of motion and control the gaps between the droplet and the neighboring walls. In addition, the point $\theta = \pi/2$ is also important. However, an examination of the system of linear algebraic equations in Eq. [A15] shows that this matrix equation becomes singular if these points are used. To overcome this difficulty, these points are replaced by closely adjacent points, i.e., $\theta=\delta$, $\pi/2-\delta$, $\pi/2+\delta$, and $\pi-\delta$. Additional points along the boundary are selected as mirror-image pairs about the plane $\theta=\pi/2$ to divide the two quarter-circular arcs of the droplet into equal segments. The optimum value of δ in this work is found to be 0.1°, with which the numerical results of the hydrodynamic drag force acting on the droplet converge satisfactorily. In selecting the boundary points, any value of ϕ may be used except $\phi=0$, $\pi/2$, and π, since the matrix equation [A15] is singular for these values.

The collocation solutions of the hydrodynamic drag force exerted on a fluid droplet translating parallel to a single plane wall (with $c\to\infty$) for various values of a/b and η^* are presented in Table A1. The drag force F_0 acting on an identical droplet in an unbounded fluid, given by Eq. [A1] (with $\mathrm{F}_0=F_0\mathrm{e}_x$), is used to normalize the boundary-corrected values. Obviously, $F/F_0=1$ as $a/b=0$ for any value of η^*. The accuracy and convergence behavior of the truncation technique depends principally upon the ratio a/b. All of the results obtained under this collocation scheme converge to at least five significant figures. For the difficult case of $a/b=0.999$, the number of collocation points $N=36$ is sufficiently large to achieve this convergence. For the special case of translation of a rigid sphere (with $\eta^*\to\infty$) parallel to a plane wall, our numerical results agree perfectly with the semianalytical solution obtained using spherical bipolar coordinates (O'Neill, 1964; Goldman *et al*., 1967). As expected, the results in Table A1. illustrate that the drag force on the droplet is a monotonically increasing function of a/b, and will become infinite in the limit $a/b=1$, for any given value of η^*. Also, the wall-corrected normalized drag force on the droplet increases monotonically with an increase in η^*, keeping a/b unchanged.

A number of converged numerical solutions for the normalized drag force F/F_0 are presented in Table A2. for the translation of a spherical droplet parallel to two plane walls at two particular positions between them (with $b/(b+c)=0.25$ and 0.5) for various values of a/b and η^* using the boundary collocation technique. For the special case of a rigid sphere (with $\eta^*\to\infty$), our results agree well with the previous solution obtained by a similar collocation method (Ganatos *et al*., 1980, in which no tabulated values are available for a precise comparison). Using a method of reflections, Shapira and Haber (1988) obtained a formula for the drag force acting on a droplet of arbitrary viscosity translating parallel to two plates to the first order of $a/(b+c)$. The values of the wall-corrected drag force calculated from this approximate formula are also listed in Table A2. for comparison. It can be seen that the method-of-reflection solution to the leading order agrees with the exact solution for small values of a/b. The errors are less than 3.7% for cases with $a/b \leq 0.2$. However, the accuracy of this approximate solution begins to deteriorate, as expected, when the droplet gets closer to the walls. For example, the errors can be greater than 12% for cases with $a/b = 0.4$. Analogous to the situation of translation parallel to a single wall, for a constant value of $b/(b+c)$, Table A2. indicates that the normalized drag force on the droplet increases monotonically with an increase in a/b (again, $F/F_0 = 1$ as $a/b = 0$) for a fixed value of η^* and with an increase in η^* for a given value of a/b.

Fig. A2 shows the drag force exerted on a gas bubble (with $\eta^* \to 0$) translating parallel to two plane walls. The dashed curves (with $a/b =$ constant) illustrate the effect of the position of the second wall (at $z = c$) on the drag for various values of the sphere-to-wall spacing b/a. The solid curves (with $2a/(b+c) =$ constant) indicate the variation of the drag force as a function of the sphere position at various values of the wall-to-wall spacing $(b+c)/2a$. At a given value of $2a/(b+c)$, the bubble (or a droplet with a finite value of η^*, whose result is not exhibited here but can also be obtained accurately) experiences minimum drag when it is located midway between the two walls, analogous to the corresponding case of a solid sphere (Ganatos *et al.*, 1980). The drag force becomes infinite as the bubble (or a droplet with finite η^*) approaches either of the walls.

In Fig. A3, the normalized drag force on a spherical droplet translating on the midplane between two parallel plane walls (with $c = b$) is plotted by solid curves as a function of a/b for various values of η^*. The corresponding drag on the droplet when the second wall is not present (with $c \to \infty$) is also plotted by dashed curves in the same figure for comparison. It can be seen from this figure (or from a comparison between Table A1. and Table A2.) that, for an arbitrary combination of parameters a/b and η^*, the assumption that the results for two walls can be obtained by simple addition of the single-wall effect gives too large a correction to the hydrodynamic drag on a droplet if

a/b is small (say, < 0.25) but underestimates the wall correction if a/b is relatively large (say, > 0.35).

A.4 Concluding remarks

In this appendix the slow motion of a spherical droplet parallel to two plane walls at an arbitrary position between them is studied theoretically. A semianalytical method with the boundary collocation technique has been used to solve the Stokes equations for the velocity fields in the fluid phases. The results for the hydrodynamic drag force exerted on the droplet indicate that the solution procedure converges rapidly and accurate solutions can be obtained for various cases of the relative viscosity of the droplet and the separation between the droplet and the walls. It has been found that, for a given relative position of the walls, the wall-corrected drag acting on the droplet normalized by the value in the absence of the walls is a monotonically increasing function of the ratio of viscosity between the internal and surrounding fluids. For a given droplet translating between two parallel walls separated by a fixed distance, the droplet experiences minimum drag when it is located midway between the walls, and the drag becomes infinite as the droplet touches either of the walls.

In Tables A1. and A2. as well as Figs. A2 and A3, we presented only the results for resistance problems, defined as those in which the drag force F acting on the droplet is to be determined for a specified droplet velocity U $[= -(F_0/6\pi\eta a)(3\eta^* + 3)/(3\eta^* + 2)]$. In a mobility problem, on the other hand, the applied force F $[= 6\pi\eta a U_0 (3\eta^* + 2)/(3\eta^* + 3)]$ exerted on the droplet is specified and the droplet velocity U is to be determined. For the creeping motion of a spherical droplet with a finite viscosity located between two parallel planes considered in this work, the ratio U/U_0 for a mobility problem equals the ratio $(F/F_0)^{-1}$ for its corresponding resistance problem. Thus, our results can also be applied to physical problems in which the force on the droplet is the prescribed quantity and the droplet must move accordingly.

Table A1. The normalized drag force F/F_0 experienced by a spherical droplet translating parallel to a single plane wall at various values of a/b and η^*

	F/F_0			
a/b	$\eta^*=0$	$\eta^*=1$	$\eta^*=10$	$\eta^*=\infty$
0.1	1.0390	1.0491	1.0576	1.0595
0.2	1.0812	1.1030	1.1217	1.1259
0.3	1.1273	1.1625	1.1932	1.2003
0.4	1.1783	1.2288	1.2741	1.2847
0.5	1.2358	1.3040	1.3675	1.3828
0.6	1.3028	1.3918	1.4790	1.5006
0.7	1.3847	1.4988	1.6191	1.6503
0.8	1.4948	1.6399	1.8109	1.8591
0.9	1.6776	1.8601	2.1262	2.2152
0.95	1.8620	2.0610	2.4255	2.5725
0.975	2.0425	2.2417	2.6978	2.9225
0.99	2.2324	2.4236	2.9759	3.3347
0.995	2.3205	2.5080	3.1100	3.5821
0.999	2.4030	2.5883	3.2439	3.9048

Table A2. The normalized drag force F/F_0 experienced by a spherical droplet translating parallel to two plane walls at various values of a/b, s ($=b/(b+c)$), and η^*

s	a/b	F/F_0			
		$\eta^*=0$	$\eta^*=1$	$\eta^*=10$	$\eta^*=\infty$
0.25	0.1	1.0455 (1.0435)	1.0574 (1.0544)	1.0674 (1.0633)	1.0697 (1.0653)
	0.2	1.0954(1.0870)	1.1215 (1.1088)	1.1438 (1.1266)	1.1489 (1.1306)
	0.3	1.1505 (1.1305)	1.1931 (1.1632)	1.2304 (1.1899)	1.2391 (1.1958)
	0.4	1.2121 (1.1740)	1.2737 (1.2175)	1.3295 (1.2531)	1.3427 (1.2611)
	0.5	1.2821 (1.2175)	1.3657 (1.2719)	1.4445 (1.3164)	1.4635 (1.3263)
	0.6	1.3637 (1.2611)	1.4730 (1.3263)	1.5812 (1.3797)	1.6080 (1.3916)
	0.7	1.4628(1.3046)	1.6024 (1.3807)	1.7504 (1.4430)	1.7884 (1.4568)
	0.8	1.5931 (1.3481)	1.7689 (1.4351)	1.9756(1.5063)	2.0322 (1.5221)
	0.9	1.8000(1.3916)	2.0178 (1.4895)	2.3294 (1.5696)	2.4278 (1.5874)
	0.95	1.9979	2.2342	2.6501	2.8067
	0.975	2.1858	2.4227	2.9337	3.1677
	0.99	2.3802	2.6093	3.2192	3.5870
	0.995	2.4699	2.6952	3.3562	3.8367
	0.999	2.5536	2.7767	3.4926	4.1613

(To be continued)

s	a/b	F/F_0			
		$\eta^* = 0$	$\eta^* = 1$	$\eta^* = 10$	$\eta^* = \infty$
0.5	0.1	1.0717 (1.0669)	1.0911 (1.0837)	1.1074 (1.0974)	1.1111 (1.1004)
	0.2	1.1546 (1.1339)	1.1986 (1.1674)	1.2373 (1.1947)	1.2462 (1.2008)
	0.3	1.2513 (1.2008)	1.3256 (1.2510)	1.3935 (1.2921)	1.4096 (1.3012)
	0.4	1.3659 (1.2678)	1.4758 (1.3347)	1.5812 (1.3895)	1.6068 (1.4016)
	0.5	1.5040 (1.3347)	1.6547 (1.4184)	1.8074 (1.4868)	1.8458 (1.5021)
	0.6	1.6748 (1.4016)	1.8709 (1.5021)	2.0840 (1.5842)	2.1395 (1.6025)
	0.7	1.8939 (1.4686)	2.1340 (1.5857)	2.4324 (1.6816)	2.5124 (1.7029)
	0.8	2.1939 (1.5355)	2.4925 (1.6694)	2.9001 (1.7790)	3.0194 (1.8033)
	0.9	2.6733 (1.6025)	3.0239 (1.7531)	3.6336 (1.8763)	3.8369 (1.9037)
	0.95	3.1154	3.4801	4.2925	4.6101
	0.975	3.5181	3.8711	4.8709	5.3405
	0.99	3.9244	4.2535	5.4513	6.1841
	0.995	4.1096	4.4287	5.7303	6.6854
	0.999	4.2818	4.5942	6.0090	7.3358

[#]The values in parentheses are calculated from the approximate formula obtained by Shapira and Haber (1988) using the method of reflections.

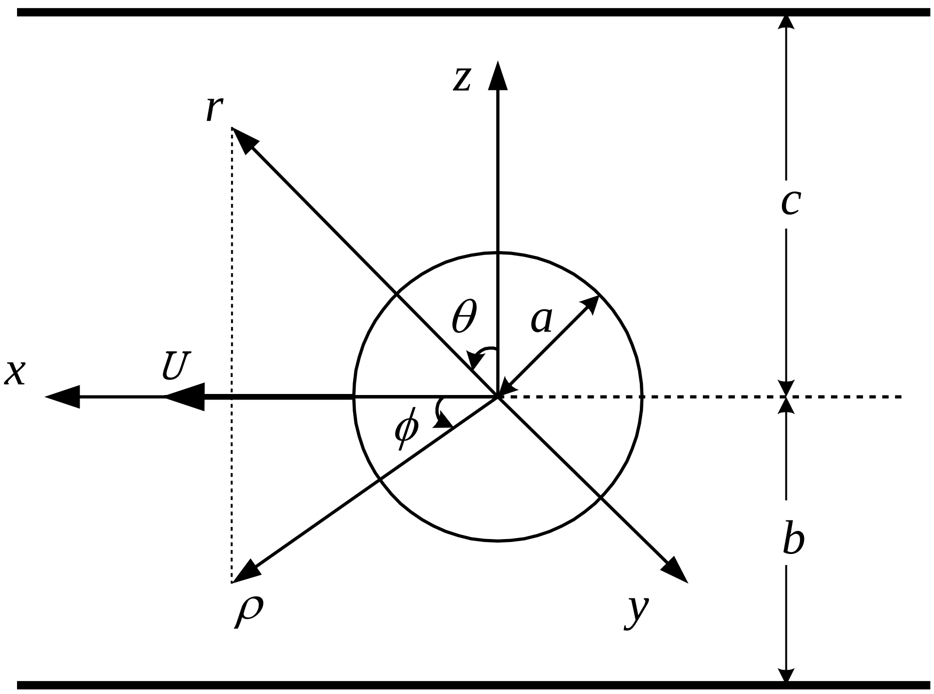

Fig. A1. Geometric sketch of the translation of a spherical droplet (particle) parallel to two plane walls at an arbitrary position between them.

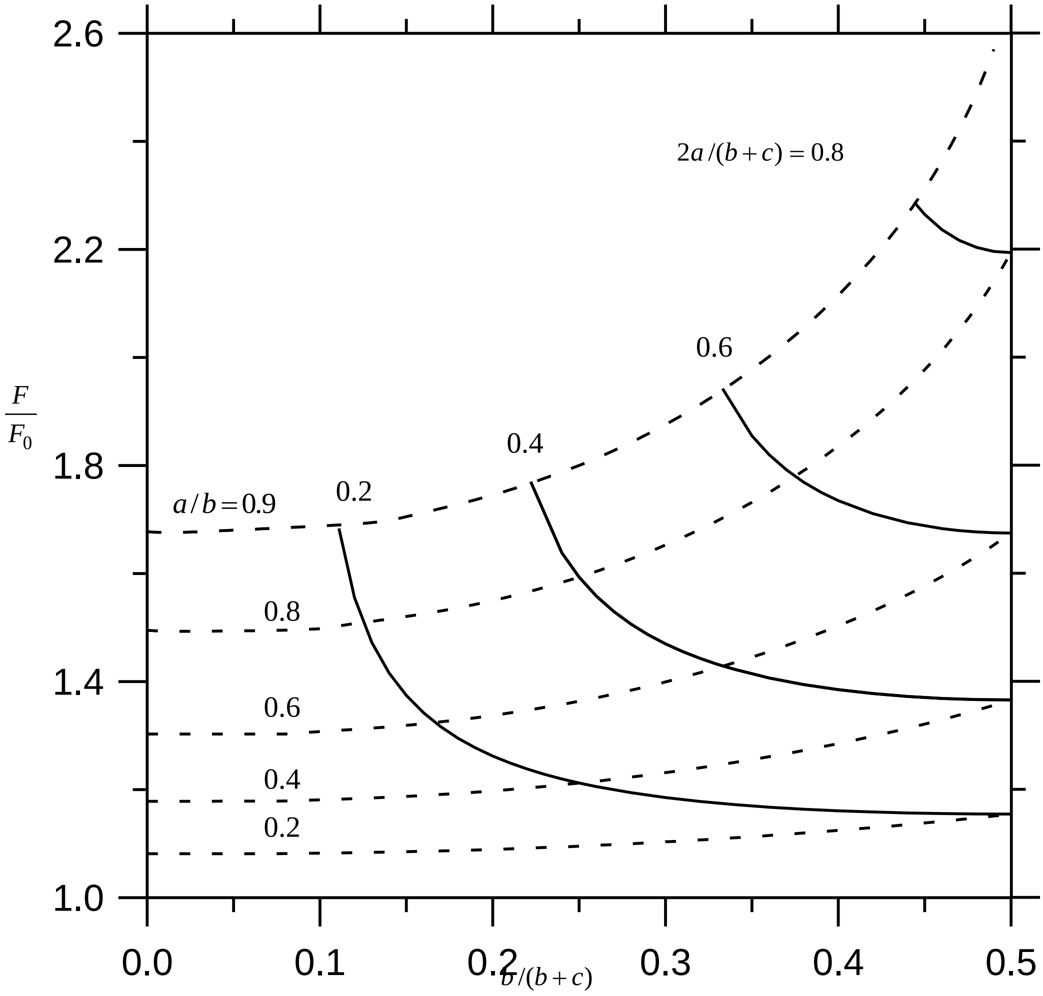

Fig. A2. Plots of the normalized drag force F/F_0 on a spherical gas bubble (with $\eta^* \to 0$) translating parallel to two plane walls versus the ratio $b/(b+c)$ with a/b and $2a/(b+c)$ as parameters.

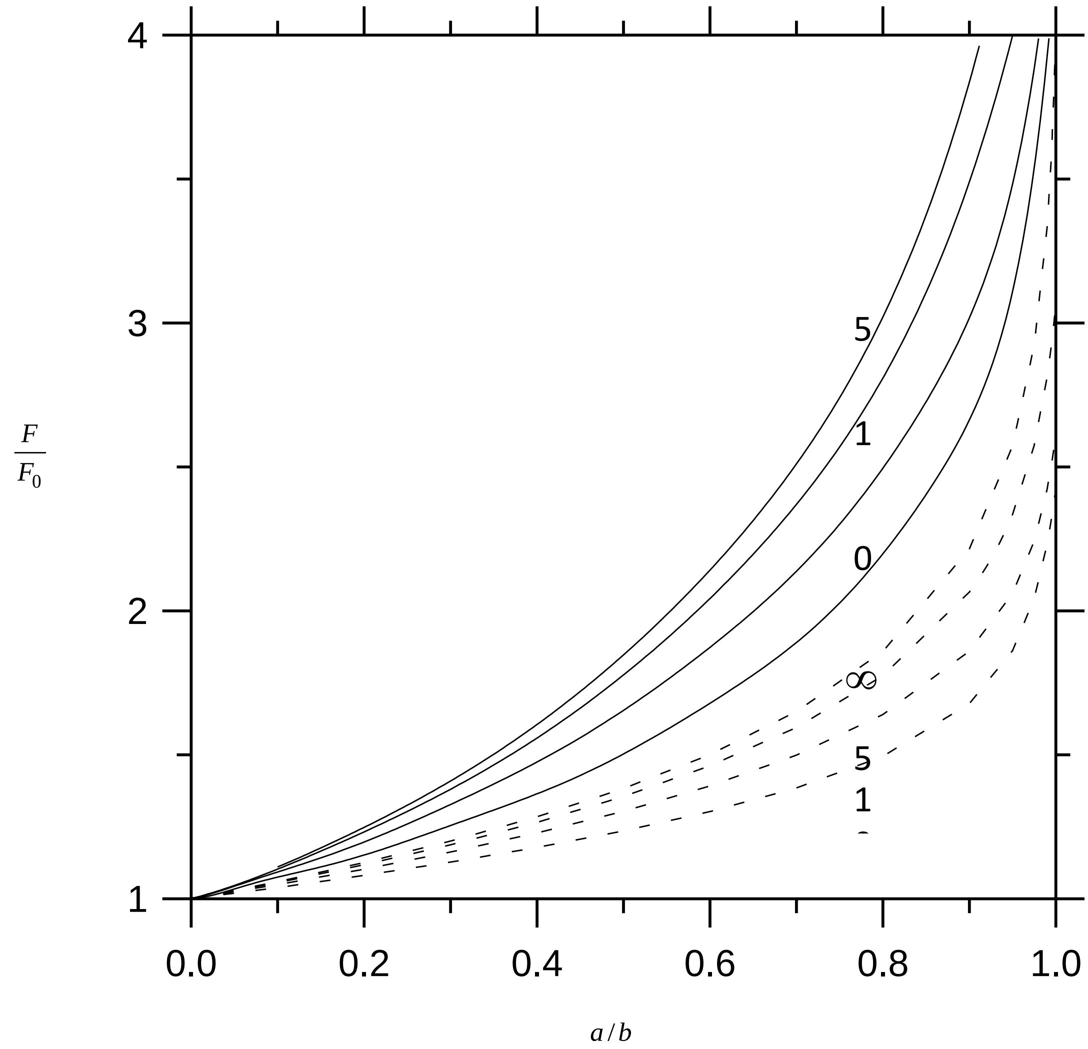

Fig. A3. Plots of the normalized drag force F/F_0 on a spherical droplet translating on the midplane between two parallel plane walls (with $c = b$) versus the ratio a/b with η^* as a parameter. The dashed curves are plotted for the translation of an identical droplet parallel to a single plane wall for comparison.

References

Bart, E., 1968. The slow unsteady settling of a fluid sphere toward a flat fluid interface. *Chem. Engng Sci.*, **23**, 193.

Brenner, H., 1961. The slow motion of a sphere through a viscous fluid towards a plane surface. *Chem. Engng Sci.*, **16**, 242.

Brenner, H., 1971. Pressure drop due to the motion of neutrally buoyant particles in duct flows. II. Spherical droplets and bubbles. *Industrial & Engng. Chem. Fundamentals*, **10**, 537.

Chen, S. B., Ye. X., 2000. Boundary effect on slow motion of a composite sphere perpendicular to two parallel impermeable plates. *Chem. Engng. Sci.*, **55**, 2441.

Coutanceau, M., Thizon, P., 1981. Wall effect on the bubble behaviour in highly viscous liquids. *J. Fluid Mech.*, **107**, 339.

Dandy, D. S., Leal, L. G., 1989. Bouyancy-driven motion of a deformable drop through a quiescent liquid at intermediate Reynolds numbers. *J. Fluid Mech.*, **208**, 161.

Ganatos, P., Weinbaum, S., Pfeffer, R., 1980. A strong interaction theory for the creeping motion of a sphere between plane parallel boundaries. Part 2. Parallel motion. *J. Fluid Mech.* **99**, 755.

Goldman, A. J., Cox, R. G., Brenner, H., 1967. Slow viscous motion of a sphere parallel to a plane wall- I. Motion through a quiescent fluid. *Chem. Engng. Sci.*, **22**, 637.

Hadamard, J. S., 1911. Mouvement permanent lent d'une sphere liquide et visqueuse dans un liquid visqueux. *Compt. Rend. Acad. Sci. (Paris)*, **152**, 1735.

Hetsroni, G., Haber, S., 1970. The flow in and around a droplet or bubble submerged in an unbound arbitrary velocity field. *Rheol. Acta.*, **9**, 488.

Keh, H. J., Tseng, Y. K., 1992. Slow motion of multiple droplets in arbitrary three-dimensional configurations. *AIChE J*, **38**, 1881.

Maude, A. D., 1961. End effects in a falling-sphere viscometer. *Britain Journal of Applied Physics*, **12**, 293.

O'Brien, V., 1968. Form factors for deformed spheroids in Stokes flow. *AIChE J* **14**, 870.

O'Neill, M. E., 1964. A slow motion of viscous liquid caused by a slowly moving solid sphere. *Mathematika*, **11**, 67.

Rushton, E., Davies, G. A., 1973. The slow unsteady settling of two fluid spheres along their line of centres. *Applied Scientific Research*, **28**, 37.

Rybczynski, W., 1911. Uber die fortschreitende bewegung einer flussigen kugel in einem zahen medium. *Bull. Acad. Sci. Cracovie Ser. A,* **1**, 40.

Shapira, M., Haber, S., 1988. Low Reynolds number motion of a droplet between two parallel plates. *Int. J. Multiphase Flow*, **14**, 483.

Taylor, T. D., Acrivos, A. 1964. On the deformation and drag of a falling viscous drop at low Reynolds number. *J. Fluid Mech.*, **18**, 466.

Wacholder, E., Weihs, D. 1972. Slow motion of a fluid sphere in the vicinity of another sphere or a plane boundary. *Chem. Engng. Sci.*, **27**, 1817.

Appendix B: the slow motion of the surface spherical particle parallel plate

B.1 Introduction

The area of the moving of solid particles or fluid drops in a continuous medium at very small Reynolds number has continued to receive much attention from investigators in the fields of chemical, biochemical, and environmental engineering and science. The majority of these moving phenomena are fundamental in nature, but permit one to develop rational understanding of many practical systems and industrial processes such as sedimentation, flotation, spray drying, agglomeration, and motion of blood cells in an artery or vein.

The theoretical study of this subject has grown out of the classic work of Stokes (1851) for a translating rigid sphere in a viscous fluid. Hadamard (1911) and Rybczynski (1911) extended independently this result to the translation of a fluid sphere. Assuming continuous velocity and continuous tangential stress across the interface of fluid phases, they found that the force exerted on a spherical drop of radius *a* by the surrounding fluid of η is

$$F = -6\pi\eta a \frac{3\eta^* + 2}{3\eta^* + 3} U, \qquad \text{[B1]}$$

Here **U** is the migration velocity of the drop and η^* is the internal-to-external viscosity ratio. Since the fluid properties are arbitrary, Eq. [B1] degenerates to the case of translation of a solid sphere (Stokes' law) when $\eta^* \to \infty$ and to the case of motion of a gas bubble with spherical shape in the limit $\eta^* \to 0$.

In most practical applications, particles or drops are not isolated. So, it is important to determine if the presence of neighboring particles and/or boundaries significantly affects the movement of particles. Problems of the hydrodynamic interactions between two or more particles and between particles and boundaries for arbitrary values of η^* have been treated extensively in the past. Summaries for the current state of knowledge in this area and some informative references can be found in Kim and Karrila (1991) and Keh and Chen (2001).

When one tries to solve the Navier-Stokes equation, it is usually assumed that no slippage arises at the solid-fluid interfaces. Actually, this is an idealization of occurrence of the transport processes. That the adjacent fluid (especially if the fluid is a rarefied gas) can slip over a solid surface has been confirmed, both experimentally and theoretically (Kennard, 1938; Loyalka, 1990; Ying and Peters, 1991; Hutchins *et al.*, 1995). Presumably any such slipping would be proportional to the local velocity gradient next to the solid surface (see Eq. [B5]), at least so long as this gradient is small (Happel and Brenner, 1983). The constant of proportionality, $1/\bar{\beta}$, may be termed a "slip coefficient." Basset (1961) derived the following expressions for the force and torque exerted by the fluid on a translating and rotating rigid sphere with a slip-flow boundary condition at its surface (e.g., an aerosol sphere):

$$F = -6\pi\eta a \frac{\bar{\beta} a + 2\eta}{\bar{\beta} a + 3\eta} U, \qquad \text{[B2a]}$$

$$\mathbf{T} = -8\pi\eta a^3 \frac{\bar{\beta} a}{\bar{\beta} a + 3\eta} \mathbf{\Omega} . \qquad \text{[B2b]}$$

Here $\mathbf{U}$ and $\mathbf{\Omega}$ are the translational and angular velocities, respectively, of the particle. In the particular case of $\bar{\beta} \to \infty$, there is no slip at the particle surface and Eq. [B2a] degenerates to Stokes' law. When $\bar{\beta} = 0$, there is a perfect slip at the particle surface and Eq. [B2a] is consistent with Eq. [B1] (taking $\eta^* = 0$). Note that, as can be seen from Eqs. [B1] and [B2a], the flow field caused by the migration of a "slip" solid sphere is the same as the external flow field generated by the same motion of a fluid drop with a value of η^* equal to $\bar{\beta} a / 3\eta$.

The slip coefficient has been determined experimentally and found to agree with the general kinetic theory of gases. It can be calculated from the formula

$$\frac{\eta}{\bar{\beta}} = C_{\mathrm{m}} l , \qquad \text{[B3]}$$

where l is the mean free path of a gas molecule and C_{m} is a dimensionless constant related to the momentum accommodation coefficient at the solid surface. Although C_{m} surely depends upon the nature of the surface, examination of the experimental data suggests that it will be in the range 1.0-1.5 (Davis, 1972; Talbot *et al*., 1980; Loyalka, 1990). Note that the slip-flow boundary condition is not only applicable in the continuum regime (the Knudsen number $l/a \ll 1$), but also appears to be valid for some cases even into the molecular flow regime ($l/a \geq 1$).

The interaction between two solid particles with finite values of $\bar{\beta} a / \eta$ is different, both physically and mathematically, from that between two fluid drops of finite viscosities. Through an exact representation in spherical bipolar coordinates, Reed and Morrison (1974) and Chen and Keh (1995a) examined the creeping motion of two rigid spheres with slip surfaces along the line of their centers. They also investigated the slow motion of a rigid sphere normal to an infinite plane wall, where the fluid may slip at the solid surfaces. Numerical results to correct Eq. [B2a] were obtained for various cases. On the other hand, the quasisteady translation and rotation of a slip spherical particle located at the center of a spherical cavity have been analyzed (Keh and Chang, 1998). Closed-form expressions for the wall-corrected drag force and torque exerted on the particle were derived.

The object of this appendix is to obtain exact solutions for the slow translational and rotational motions of a spherical particle with a slip surface parallel to two plane walls at an arbitrary position between them. The creeping-flow equations applicable to the system are solved by using a combined analytical-numerical method with a boundary collocation technique (Ganatos *et al*., 1980) and the wall-corrected drag and torque acting on the particle are obtained with good convergence for various cases. For the special cases of movement of a particle with zero and infinite slip coefficients, our calculations show excellent agreement with the available solutions in the literature for the corresponding motions of a no-slip solid sphere and of a gas bubble, respectively.

B.2 Analysis

We consider the steady creeping motion caused by a rigid spherical particle of radius *a* translating with a velocity $\mathbf{U} = U\mathbf{e}_x$ and rotating with an angular velocity $\mathbf{\Omega} = \Omega\mathbf{e}_y$ in a gaseous medium parallel to two infinite plane walls whose distances from the center of the particle are *b* and *c*, as shown in

Figure A1. Here (x, y, z), (ρ, ϕ, z), and (r, θ, ϕ) denote the rectangular, circular cylindrical, and spherical coordinate systems, respectively, with the origin of coordinates at the particle center, and $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$ are the unit vectors in rectangular coordinates. We set $b \le c$ throughout this work, without the loss of generality. The fluid is at rest far away from the particle. It is assumed that the Knudsen number l/a is small so that the fluid flow is in the continuum regime and the Knudsen layer at the particle surface is thin in comparison with the radius of the particle and the spacing between the particle and each wall. The objective is to determine the correction to Eq. [B2] for the motion of the particle due to the presence of the plane walls.

The fluid is assumed to be incompressible and Newtonian. Owing to the low Reynolds number, the fluid motion is governed by the Stokes equations,

$$\eta \nabla^2 \mathbf{v} - \nabla p = 0 , \qquad \text{[B4a]}$$

$$\nabla \cdot \mathbf{v} = 0 , \qquad \text{[B4b]}$$

where $\mathbf{v}(\mathbf{x})$ is the velocity field for the fluid flow and $p(\mathbf{x})$ is the dynamic pressure distribution.

The boundary conditions for the fluid velocity at the particle surface, on the plane walls, and far removed from the particle are

$$r = a: \qquad \mathbf{v} = \mathbf{U} + a\boldsymbol{\Omega} \times \mathbf{e}_r + \frac{1}{\overline{\beta}} (\mathbf{I} - \mathbf{e}_r \mathbf{e}_r)\mathbf{e}_r : \boldsymbol{\tau} , \qquad \text{[B5]}$$

$$z = c, -b: \qquad \mathbf{v} = 0 , \qquad \text{[B6]}$$

$$\rho \to \infty: \qquad \mathbf{v} = 0 . \qquad \text{[B7]}$$

Here, $\boldsymbol{\tau} = \eta[\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}}]$ is the viscous stress tensor for the fluid, $\mathbf{e}_r$ together with $\mathbf{e}_\theta$ and $\mathbf{e}_\phi$ are the unit vectors in spherical coordinates, $\mathbf{I}$ is the unit dyadic, and $1/\overline{\beta}$ is the frictional slip coefficient about the surface of the particle.

A fundamental solution to Eq. [B4] which satisfies Eqs. [B6] and [B7] is

$$\mathbf{v} = v_x \mathbf{e}_x + v_y \mathbf{e}_y + v_z \mathbf{e}_z , \qquad \text{[B8]}$$

where

$$v_x = \sum_{n=1}^{\infty} [A_n (A'_n + \alpha'_n) + B_n (B'_n + \beta'_n) + C_n (C'_n + \gamma'_n)] , \qquad \text{[B9a]}$$

$$v_y = \sum_{n=1}^{\infty} [A_n (A''_n + \alpha''_n) + B_n (B''_n + \beta''_n) + C_n (C''_n + \gamma''_n)] , \qquad \text{[B9b]}$$

$$v_z = \sum_{n=1}^{\infty} [A_n (A'''_n + \alpha'''_n) + B_n (B'''_n + \beta'''_n) + C_n (C'''_n + \gamma'''_n)] . \qquad \text{[B9c]}$$

Here, the primed A_n, B_n, C_n, α_n, β_n, and γ_n are functions of position involving associated Legendre functions of $\mu = \cos\theta$ defined by Eq. [2.6] and in the form of integration (which must be performed numerically) defined by Eq. [C1] of Ganatos *et al*. (1980), and A_n, B_n, and C_n are unknown constants.

The boundary condition that remains to be satisfied is that on the particle surface. Substituting Eq. [B8] into Eq. [B5], one obtains

$$\sum_{n=1}^{\infty}[A_n A_n^{*}(a,\mu,\phi)+B_n B_n^{*}(a,\mu,\phi)+C_n C_n^{*}(a,\mu,\phi)]=U(1-\mu^2)^{1/2}\cos\phi\,, \tag{B10a}$$

$$\begin{aligned}
&\sum_{n=1}^{\infty}[A_n A_n^{**}(a,\mu,\phi)+B_n B_n^{**}(a,\mu,\phi)+C_n C_n^{**}(a,\mu,\phi)] \\
&\quad -\frac{\eta}{\overline{\beta}a}\sum_{n=1}^{\infty}\{(r\frac{\partial}{\partial r}-1)[A_n A_n^{**}(r,\mu,\phi)+B_n B_n^{**}(r,\mu,\phi)+C_n C_n^{**}(r,\mu,\phi)] \\
&\quad -(1-\mu^2)^{1/2}\frac{\partial}{\partial\mu}[A_n A_n^{*}(r,\mu,\phi)+B_n B_n^{*}(r,\mu,\phi)+C_n C_n^{*}(r,\mu,\phi)]\}_{r=a} \\
&\quad = U\mu\cos\phi + a\Omega\cos\phi\,,
\end{aligned} \tag{B10b}$$

$$\begin{aligned}
&\sum_{n=1}^{\infty}[A_n A_n^{***}(a,\mu,\phi)+B_n B_n^{***}(a,\mu,\phi)+C_n C_n^{***}(a,\mu,\phi)] \\
&\quad -\frac{\eta}{\overline{\beta}a}\sum_{n=1}^{\infty}\{(r\frac{\partial}{\partial r}-1)[A_n A_n^{***}(r,\mu,\phi)+B_n B_n^{***}(r,\mu,\phi)+C_n C_n^{***}(r,\mu,\phi)] \\
&\quad +(1-\mu^2)^{-1/2}\frac{\partial}{\partial\phi}[A_n A_n^{*}(r,\mu,\phi)+B_n B_n^{*}(r,\mu,\phi)+C_n C_n^{*}(r,\mu,\phi)]\}_{r=a} \\
&\quad = -U\sin\phi - a\Omega\mu\sin\phi\,.
\end{aligned} \tag{B10c}$$

The starred A_n, B_n, and C_n functions in Eq. [B10] are defined by

$$A_n^{*}(r,\mu,\phi)=(1-\mu^2)^{1/2}(A_n'+\alpha_n')\cos\phi+(1-\mu^2)^{1/2}(A_n''+\alpha_n'')\sin\phi+\mu(A_n'''+\alpha_n''')\,, \tag{B11a}$$

$$B_n^{*}(r,\mu,\phi)=(1-\mu^2)^{1/2}(B_n'+\beta_n')\cos\phi+(1-\mu^2)^{1/2}(B_n''+\beta_n'')\sin\phi+\mu(B_n'''+\beta_n''')\,, \tag{B11b}$$

$$C_n^{*}(r,\mu,\phi)=(1-\mu^2)^{1/2}(C_n'+\gamma_n')\cos\phi+(1-\mu^2)^{1/2}(C_n''+\gamma_n'')\sin\phi+\mu(C_n'''+\gamma_n''')\,, \tag{B11c}$$

$$A_n^{**}(r,\mu,\phi)=\mu(A_n'+\alpha_n')\cos\phi+\mu(A_n''+\alpha_n'')\sin\phi-(1-\mu^2)^{1/2}(A_n'''+\alpha_n''')\,, \tag{B11d}$$

$$B_n^{**}(r,\mu,\phi)=\mu(B_n'+\beta_n')\cos\phi+\mu(B_n''+\beta_n'')\sin\phi-(1-\mu^2)^{1/2}(B_n'''+\beta_n''')\,, \tag{B11e}$$

$$C_n^{**}(r,\mu,\phi)=\mu(C_n'+\gamma_n')\cos\phi+\mu(C_n''+\gamma_n'')\sin\phi-(1-\mu^2)^{1/2}(C_n'''+\gamma_n''')\,, \tag{B11f}$$

$$A_n^{***}(r,\mu,\phi)=-(A_n'+\alpha_n')\sin\phi+(A_n''+\alpha_n'')\cos\phi\,, \tag{B11g}$$

$$B_n^{***}(r,\mu,\phi)=-(B_n'+\beta_n')\sin\phi+(B_n''+\beta_n'')\cos\phi\,, \tag{B11h}$$

$$C_n^{***}(r,\mu,\phi)=-(C_n'+\gamma_n')\sin\phi+(C_n''+\gamma_n'')\cos\phi\,, \tag{B11i}$$

where the primed A_n, B_n, C_n, α_n, β_n, and γ_n are functions of position in Eq. [B9].

Careful examination of Eq. [B10] shows that the solution of the coefficient matrix generated is independent of the ϕ coordinate of the boundary points on the surface of the sphere $r = a$. To satisfy the conditions in Eq. [B10] exactly along the entire surface of the particle would require the solution of the entire infinite array of unknown constants A_n, B_n, and C_n. However, the collocation method (O'Brien, 1968; Ganatos *et al*., 1980) enforces the boundary conditions at a finite number of discrete points on the half-circular generating arc of the sphere (from $\theta = 0$ to $\theta = \pi$) and truncates the infinite series in Eq. [B9] into finite ones. If the spherical boundary is approximated by satisfying the conditions of Eq. [B10] at *N* discrete points on its generating arc, the infinite series in Eq. [B9] are truncated after *N* terms, resulting in a system of *3N* simultaneous linear algebraic equations in the truncated form of Eq. [B10]. This matrix equation can be numerically solved to yield the 3*N* unknown constants A_n, B_n, and C_n required in the truncated form of Eq. [B9]. The fluid velocity field is completely obtained once these coefficients are solved for a sufficiently large value of *N*. The accuracy of the boundary-collocation/truncation technique can be improved to any degree by taking a sufficiently large value of *N*. Naturally, as $N \to \infty$ the truncation error vanishes and the overall accuracy of the solution depends only on the numerical integration required in evaluating the matrix elements.

The drag force $\mathrm{F} = F\,\mathrm{e}_x$ and torque $\mathrm{T} = T\,\mathrm{e}_y$ exerted by the fluid on the spherical particle about its center can be determined from (Ganatos *et al*., 1980)

$$F = -8\pi\eta\, A_1, \quad \text{[B12a]}$$

$$T = -8\pi\eta\, C_1\,. \quad \text{[B12b]}$$

These expressions show that only the lowest-order coefficients A_1 and C_1 contribute to the hydrodynamic force and couple acting on the particle. Equation [B12] can also be expressed in terms of the translational and angular velocities of the particle as

$$F = -6\pi\eta a \frac{\overline{\beta}a + 2\eta}{\overline{\beta}a + 3\eta}(UF_\mathrm{t} + a\Omega F_\mathrm{r})\,, \quad \text{[B13a]}$$

$$T = -8\pi\eta a^2 \frac{\overline{\beta}a}{\overline{\beta}a + 3\eta}(UT_\mathrm{t} + a\Omega T_\mathrm{r})\,, \quad \text{[B13b]}$$

where F_t, F_r, T_t, and T_r are nondimensional force and torque coefficients to be calculated using the results of A_1 and C_1. According to the cross-effect theory for the force and torque on a rigid particle in quasistatic Stokes motion near a rigid boundary (Goldman *et al*., 1967), it can be shown that the coupling coefficients F_r and T_t satisfy the relation

$$T_\mathrm{t} = \frac{3}{4}\frac{\overline{\beta}a + 2\eta}{\overline{\beta}a}F_\mathrm{r}\,. \quad \text{[B14]}$$

Thus, only the collocation results of the coefficients F_t, F_r, and T_r will be presented in the following section.

B.3 Results And Discussion

The solution for the slow motion of a spherical particle parallel to two plane walls at an arbitrary position between them, obtained by using the boundary collocation method described in the previous section, is presented in this section. The system of linear algebraic equations to be solved for the coefficients A_n, B_n, and C_n is constructed from Eq. [B10]. All the numerical integrations to evaluate the primed α_n, β_n, and γ_n functions were done by the 80-point Gauss-Laguerre guadrature. The numerical calculations were performed by using a DEC 3000/600 workstation.

When specifying the points along the semicircular generating arc of the sphere (with a constant value of ϕ) where the boundary conditions are to be exactly satisfied, the first points that should be chosen are $\theta = 0$ and π, since these points define the projected area of the particle normal to the direction of motion and control the gaps between the particle and the neighboring plates. In addition, the point $\theta = \pi/2$ is also important. However, an examination of the system of linear algebraic equations in Eq. [B10] shows that the matrix equations become singular if these points are used. To overcome this difficulty, these points are replaced by closely adjacent points, i.e., $\theta = \delta$, $\pi/2 - \delta$, $\pi/2 + \delta$, and $\pi - \delta$ (Ganatos *et al*., 1980). Additional points along the boundary are selected as mirror-image pairs about the plane $\theta = \pi/2$ to divide the two quarter-circular arcs of the particle into equal segments. The optimum value of δ in this work is found to be 0.1°, with which the numerical results of the hydrodynamic drag force and torque acting on the particle converge satisfactorily. In selecting the boundary points, any value of ϕ may be used except for $\phi = 0, \pi/2$, and π since the matrix equation [B10] is singular for these values.

The collocation solutions of the dimensionless force and torque coefficients for the translation and rotation of a spherical particle parallel to a plane wall (with $c \to \infty$) for different values of the parameters $\bar{\beta}a/\eta$ and a/b are presented in Tables B1-B3. Obviously, $F_t = T_r = 1$ and $F_r = T_t = 0$ as $a/b = 0$ for any value of $\bar{\beta}a/\eta$. All of the results obtained under the collocation scheme converge satisfactorily to at least the significant figures shown in the tables. The accuracy and convergence behavior of the truncation technique is principally a function of the ratio a/b. For the most difficult case with $a/b = 0.999$, the number of collocation points $N = 42$ is sufficiently large to achieve this convergence. For the special case of translation and rotation of a no-slip sphere (with $\bar{\beta}a/\eta \to \infty$) parallel to a plane wall, our numerical results agree perfectly with the semianalytical solution obtained using spherical bipolar coordinates (Dean and O'Neill, 1963; O'Neill, 1964; Goldman *et al*., 1967). For the other particular case of translaion of a perfectly-slip sphere (with $\bar{\beta}a/\eta = 0$) parallel to a plane wall, our results (given in Table B1) are also in perfect agreement with the boundary-collocation solution obtained for the migration of a spherical gas bubble with $\eta^* = 0$ (Keh and Chen, 2001). As expected, the results in Tables B1 and B2 illustrate that the normalized drag force (F_t) and torque (T_r) on the particle are monotonically increasing functions of a/b, and will become infinite in the limit $a/b = 1$, for any given value of $\bar{\beta}a/\eta$. These normalized drag force and torque in general increase with an increase in $\bar{\beta}a/\eta$ (or with a decrease in the slip coefficient $\bar{\beta}^{-1}$), keeping a/b unchanged. On the other hand, as shown in Table B3, the coupling coefficients F_r and T_t are not necessarily a monotonic function of the parameter a/b or $\bar{\beta}a/\eta$, and their values can be either positive or negative depending on the combination of a/b and $\bar{\beta}a/\eta$.

A number of converged boundary-collocation solutions for the dimensionless force and torque coefficients are presented in Tables B4-B6 for the translation and rotation of a spherical particle parallel to two plane walls at two particular positions between them (with $b/(b+c)=0.25$ and 0.5) for various values of a/b and $\bar{\beta}a/\eta$. For the special cases of a no-slip sphere (with $\bar{\beta}a/\eta \to \infty$) and a perfectly-slip sphere (with $\bar{\beta}a/\eta = 0$), our results agree well with the previous solutions obtained by a similar collocation method (Ganatos *et al.*, 1980, in which no tabulated values are available for a precise comparison; Keh and Chen, 2001). Analogous to the situation of translation and rotation parallel to a single wall, for a constant value of $b/(b+c)$, Tables B4 and B5 indicate that the normalized drag force and torque on the particle increase monotonically with an increase in a/b for a fixed value of $\bar{\beta}a/\eta$ and with an increase in $\bar{\beta}a/\eta$ for a given value of a/b (with exceptions), while Table B6 shows that the coupling coefficients F_{r} and T_{t} can be either positive or negative depending on the combination of the parameters a/b and $\bar{\beta}a/\eta$. Again, $F_{\mathrm{t}} = T_{\mathrm{r}} = 1$ and $F_{\mathrm{r}} = T_{\mathrm{t}} = 0$ as $a/b = 0$ for any given values of $b/(b+c)$ and $\bar{\beta}a/\eta$.

Figures B1-B3 show the force and torque coefficients for the translation and rotation of a spherical particle with $\bar{\beta}a/\eta = 10$ parallel to two plane walls. The dashed curves (with $a/b=$ constant) illustrate the effect of the position of the second wall (at $z=c$) on the drag force and torque for various values of the sphere-to-wall spacing b/a. The solid curves (with $2a/(b+c)=$ constant) indicate the variation of the drag force and torque as functions of the sphere position at various values of the wall-to-wall spacing $(b+c)/2a$. At a given value of $2a/(b+c)$, the particle (or a particle with any other value of $\bar{\beta}a/\eta$, whose collocation results are not exhibited here but can also be obtained accurately) experiences minimum drag when it is located midway between the two walls as illustrated in Figs. B1 and B2, analogous to the corresponding cases of a no-slip sphere (Ganatos *et al.*, 1980) and of a fluid sphere (Keh and Chen, 2001). The drag force and torque become infinite as the particle approaches either of the walls. Again, Fig. B3 indicates that the coupling coefficient F_{r} (and T_{t}) is not a monotonic function of the relevant parameters.

In Figs. B4 and B5, the force and torque coefficients F_{t} and T_{r} for the motion of a spherical particle on the midplane between two parallel plane walls (with $c=b$) are plotted by solid curves as functions of a/b for various values of $\bar{\beta}a/\eta$. The corresponding drag coefficients for the particle when the second wall is not present (with $c \to \infty$) are also plotted by dashed curves in the same figures for comparison. It can be seen from these figures (or from a comparison between Tables B1 and B2 and Tables B4 and B5) that, for an arbitrary combination of parameters a/b and $\bar{\beta}a/\eta$, the assumption that the results for two walls can be obtained by simple addition of the single-wall effect gives too large a correction to the hydrodynamic drag force on a particle if a/b is small (say, <0.25) and to the torque on the particle for any value of a/b, but underestimates the drag force if a/b is relatively large (say, >0.35).

B.4 Concluding remarks

In this appendix the slow translational and rotational motions of a spherical particle parallel to two plane walls at an arbitrary position between them are studied theoretically, where the fluid may slip at the particle surface. A semi-analytical method with the boundary collocation technique has been used to solve the Stokes equations for the fluid velocity field. The results for the hydrodynamic drag force and torque exerted on the particle indicate that the solution procedure converges rapidly and accurate solutions can be obtained for various cases of the particle slip coefficient and of the separation between the particle and the walls. It has been found that, for a given relative position of the walls, the wall-corrected drag force and torque acting on the particle normalized by the values in the absence of the walls in general are decreasing functions of the slip coefficient. For a given particle translating and rotating between two parallel walls separated by a fixed distance, the particle experiences minimum drag force and couple when it is located midway between the walls, and the drag force and couple become infinite as the particle touches either of the walls.

In Tables B1-B6 and Figs. B1-B5, we presented the explicit results for resistance problems, defined as those in which the drag force **F** and hydrodynamic torque **T** acting on the particle are to be determined for specified particle velocities $\mathbf{U}$ and $\mathbf{\Omega}$. In a mobility problem, on the other hand, the applied force **F** and torque **T** exerted on the particle are specified and the particle velocities **U** and $\mathbf{\Omega}$ are to be determined. For the creeping motion of a spherical particle with a finite slip coefficient located between two parallel planes considered in this work, our results expressed by Eq. [B13] can also be used for its corresponding mobility problems in which the force and torque on the particle are the prescribed quantities and the particle must move accordingly. For example, the translational and angular velocities of a slip sphere parallel to one or two plane walls driven by an applied force $F\,\mathbf{e}_x$ under the condition of free rotation are obtained from Eq. [B13] as

$$U=\frac{F}{6\pi\eta a}\frac{\bar{\beta}a+3\eta}{\bar{\beta}a+2\eta}(F_{\mathrm{t}}-F_{\mathrm{r}}\frac{T_{\mathrm{t}}}{T_{\mathrm{r}}})^{-1}, \qquad \text{[B15a]}$$

$$\Omega=-\frac{U}{a}\frac{T_{\mathrm{t}}}{T_{\mathrm{r}}}. \qquad \text{[B15b]}$$

The values of the force and torque coefficients in Eq. [B15] are the same as those presented in Tables B1-B6 and Figs. B1-B5.

Table B1. The force coefficient F_t for the translation of a spherical particle parallel to a single plane wall at various values of a/b and $\bar{\beta}a/\eta$

a/b	F_t			
	$\bar{\beta}a/\eta=0$	$\bar{\beta}a/\eta=1$	$\bar{\beta}a/\eta=10$	$\bar{\beta}a/\eta\to\infty$
0.1	1.0390	1.0440	1.0547	1.0595
0.2	1.0812	1.0920	1.1152	1.1259
0.3	1.1273	1.1445	1.1824	1.2003
0.4	1.1783	1.2026	1.2578	1.2847
0.5	1.2358	1.2680	1.3439	1.3828
0.6	1.3028	1.3434	1.4449	1.5006
0.7	1.3847	1.4342	1.5687	1.6503
0.8	1.4948	1.5523	1.7312	1.8591
0.9	1.6776	1.7366	1.9772	2.2152
0.95	1.8620	1.9107	2.1848	2.5725
0.975	2.0425	2.0755	2.3568	2.9225
0.99	2.2324	2.2468	2.5213	3.3347
0.995	2.3205	2.3261	2.5958	3.5821
0.999	2.4030	2.4005	2.6657	3.9048

Table B2. The torque coefficient T_r for the rotation of a spherical particle parallel to a single plane wall at various values of a/b and $\bar{\beta}a/\eta$

a/b	T_r			
	$\bar{\beta}a/\eta=0.1$	$\bar{\beta}a/\eta=1$	$\bar{\beta}a/\eta=10$	$\bar{\beta}a/\eta\to\infty$
0.1	1.0000	1.0001	1.0002	1.0003
0.2	1.0001	1.0006	1.0019	1.0025
0.3	1.0003	1.0021	1.0066	1.0086
0.4	1.0007	1.0051	1.0158	1.0207
0.5	1.0013	1.0100	1.0316	1.0418
0.6	1.0022	1.0175	1.0570	1.0763
0.7	1.0035	1.0285	1.0965	1.1324
0.8	1.0053	1.0437	1.1590	1.2283
0.9	1.0076	1.0645	1.2655	1.4253
0.95	1.0089	1.0772	1.3524	1.6500
0.975	1.0096	1.0840	1.4112	1.8862
0.99	1.0100	1.0881	1.4526	2.1808
0.995	1.0101	1.0894	1.4672	2.3677
0.999	1.0102	1.0904	1.4790	2.6242

Table B3. The coupling coefficient $F_{\mathrm{r}} = T_{\mathrm{t}}(4/3)\bar{\beta}a/(\bar{\beta}a+2\eta)$ for the motion of a spherical particle parallel to a single plane wall at various values of a/b and $\bar{\beta}a/\eta$

a/b	F_{r}			
	$\bar{\beta}a/\eta=0.1$	$\bar{\beta}a/\eta=1$	$\bar{\beta}a/\eta=10$	$\bar{\beta}a/\eta\to\infty$
.1	-3.7E-9	-9.3E-7	-7.6E-6	-1.2E-5
0.2	2.1E-7	-1.3E-5	-1.2E-4	-1.8E-4
0.3	2.6E-6	-5.6E-5	-5.7E-4	-9.0E-4
0.4	1.4E-5	-1.4E-4	-0.0018	-0.0028
0.5	5.1E-5	-2.3E-4	-0.0042	-0.0067
0.6	1.5E-4	-2.1E-4	-0.0085	-0.0141
0.7	3.9E-4	3.2E-4	-0.0157	-0.0275
0.8	9.5E-4	0.0024	-0.0272	-0.0528
0.9	0.0023	0.0092	-0.0434	-0.1095
0.95	0.0037	0.0178	-0.0483	-0.1798
0.975	0.0047	0.0253	-0.0429	-0.2680
0.99	0.0056	0.0315	-0.0329	-0.4292
0.995	0.0059	0.0338	-0.0284	-0.5695
0.999	0.0061	0.0357	-0.0245	-0.8012

Table B4. The force coefficient F_{t} for the translation of a spherical particle parallel to two plane walls at various values of a/b, $b/(b+c)$, and $\bar{\beta}a/\eta$

$b/(b+c)$	a/b	F_{t}			
		$\bar{\beta}a/\eta=0$	$\bar{\beta}a/\eta=1$	$\bar{\beta}a/\eta=10$	$\bar{\beta}a/\eta\to\infty$
0.25	0.1	1.0455	1.0514	1.0640	1.0697
	0.2	1.0954	1.1083	1.1360	1.1489
	0.3	1.1505	1.1713	1.2173	1.2391
	0.4	1.2121	1.2419	1.3095	1.3427
	0.5	1.2821	1.3218	1.4155	1.4635
	0.6	1.3637	1.4141	1.5397	1.6080
	0.7	1.4628	1.5246	1.6901	1.7884
	0.8	1.5931	1.6654	1.8830	2.0322
	0.9	1.8000	1.8763	2.1634	2.4278
	0.95	1.9979	2.0654	2.3898	2.8067
	0.975	2.1858	2.2381	2.5718	3.1677
	0.99	2.3802	2.4143	2.7424	3.5870
	0.995	2.4699	2.4953	2.8190	3.8367
	0.999	2.5536	2.5710	2.8905	4.1613

(to be continued)

$b/(b+c)$	a/b	F_t			
		$\bar{\beta}a/\eta=0$	$\bar{\beta}a/\eta=1$	$\bar{\beta}a/\eta=10$	$\bar{\beta}a/\eta\to\infty$
0.5	0.1	1.0717	1.0813	1.1018	1.1111
	0.2	1.1546	1.1762	1.2238	1.2462
	0.3	1.2513	1.2873	1.3695	1.4096
	0.4	1.3659	1.4184	1.5432	1.6068
	0.5	1.5040	1.5745	1.7508	1.8458
	0.6	1.6748	1.7636	2.0018	2.1395
	0.7	1.8939	1.9995	2.3124	2.5124
	0.8	2.1939	2.3105	2.7158	3.0194
	0.9	2.6733	2.7817	3.3036	3.8369
	0.95	3.1154	3.1950	3.7748	4.6101
	0.975	3.5181	3.5615	4.1497	5.3405
	0.99	3.9244	3.9275	4.4984	6.1841
	0.995	4.1096	4.0942	4.6541	6.6854
	0.999	4.2818	4.2494	4.7992	7.3358

Table B5. The torque coefficient T_{r} for the rotation of a spherical particle parallel to two plane walls at various values of a/b, $b/(b+c)$, and $\bar{\beta}a/\eta$

$b/(b+c)$	a/b	T_{r}			
		$\bar{\beta}a/\eta = 0.1$	$\bar{\beta}a/\eta = 1$	$\bar{\beta}a/\eta = 10$	$\bar{\beta}a/\eta \to \infty$
0.25	0.1	1.0000	1.0001	1.0003	1.0003
	0.2	1.0001	1.0007	1.0020	1.0026
	0.3	1.0003	1.0022	1.0068	1.0089
	0.4	1.0007	1.0053	1.0164	1.0215
	0.5	1.0013	1.0104	1.0328	1.0433
	0.6	1.0023	1.0182	1.0590	1.0790
	0.7	1.0037	1.0295	1.0997	1.1365
	0.8	1.0055	1.0453	1.1636	1.2344
	0.9	1.0079	1.0666	1.2720	1.4337
	0.95	1.0092	1.0796	1.3600	1.6598
	0.975	1.0099	1.0865	1.4193	1.8968
	0.99	1.0103	1.0907	1.4611	2.1918
	0.995	1.0105	1.0921	1.4758	2.3789
	0.999	1.0106	1.0932	1.4877	2.6356

(to be continued)

$b/(b+c)$	a/b	T_r			
		$\bar{\beta}a/\eta = 0.1$	$\bar{\beta}a/\eta = 1$	$\bar{\beta}a/\eta = 10$	$\bar{\beta}a/\eta \to \infty$
0.5	0.1	1.0000	1.0001	1.0004	1.0005
	0.2	1.0001	1.0011	1.0033	1.0043
	0.3	1.0005	1.0036	1.0113	1.0147
	0.4	1.0011	1.0087	1.0273	1.0358
	0.5	1.0022	1.0172	1.0551	1.0730
	0.6	1.0038	1.0303	1.1002	1.1351
	0.7	1.0061	1.0495	1.1719	1.2381
	0.8	1.0093	1.0768	1.2877	1.4188
	0.9	1.0133	1.1145	1.4900	1.7994
	0.95	1.0157	1.1378	1.6578	2.2414
	0.975	1.0169	1.1503	1.7723	2.7100
	0.99	1.0176	1.1579	1.8532	3.2968
	0.995	1.0178	1.1604	1.8818	3.6698
	0.999	1.0180	1.1623	1.9050	4.1822

Table B6. The coupling coefficient $F_{\mathrm{r}} = T_{\mathrm{t}}(4/3)\bar{\beta}a/(\bar{\beta}a + 2\eta)$ for the motion of a spherical particle parallel to two plane walls at the position $b/(b+c) = 1/4$ * for various values of a/b and $\bar{\beta}a/\eta$

a/b	F_{r}			
	$\bar{\beta}a/\eta = 0.1$	$\bar{\beta}a/\eta = 1$	$\bar{\beta}a/\eta = 10$	$\bar{\beta}a/\eta \to \infty$
0.1	1.1E-5	8.7E-5	2.7 E-4	3.5 E-4
0.2	4.7E-5	3.6 E-4	0.0011	0.0014
0.3	1.1E-4	8.2E-4	0.0022	0.0028
0.4	2.2E-4	0.0015	0.0035	0.0041
0.5	3.9E-4	0.0024	0.0044	0.0046
0.6	6.6E-4	0.0038	0.0043	0.0028
0.7	0.0011	0.0059	0.0022	-0.0037
0.8	0.0019	0.0099	-0.0031	-0.0209
0.9	0.0035	0.0189	-0.0122	-0.0682
0.95	0.0050	0.0286	-0.0131	-0.1332
0.975	0.0062	0.0367	-0.0057	-0.2187
0.99	0.0071	0.0433	0.0055	-0.3783
0.995	0.0074	0.0457	0.0105	-0.5180
0.999	0.0076	0.0477	0.0146	-0.7492

*For the motion of a sphere on the midplane between two parallel plane walls (with $b/(b+c) = 1/2$), it is obvious that $F_{\mathrm{r}} = T_{\mathrm{t}} = 0$.

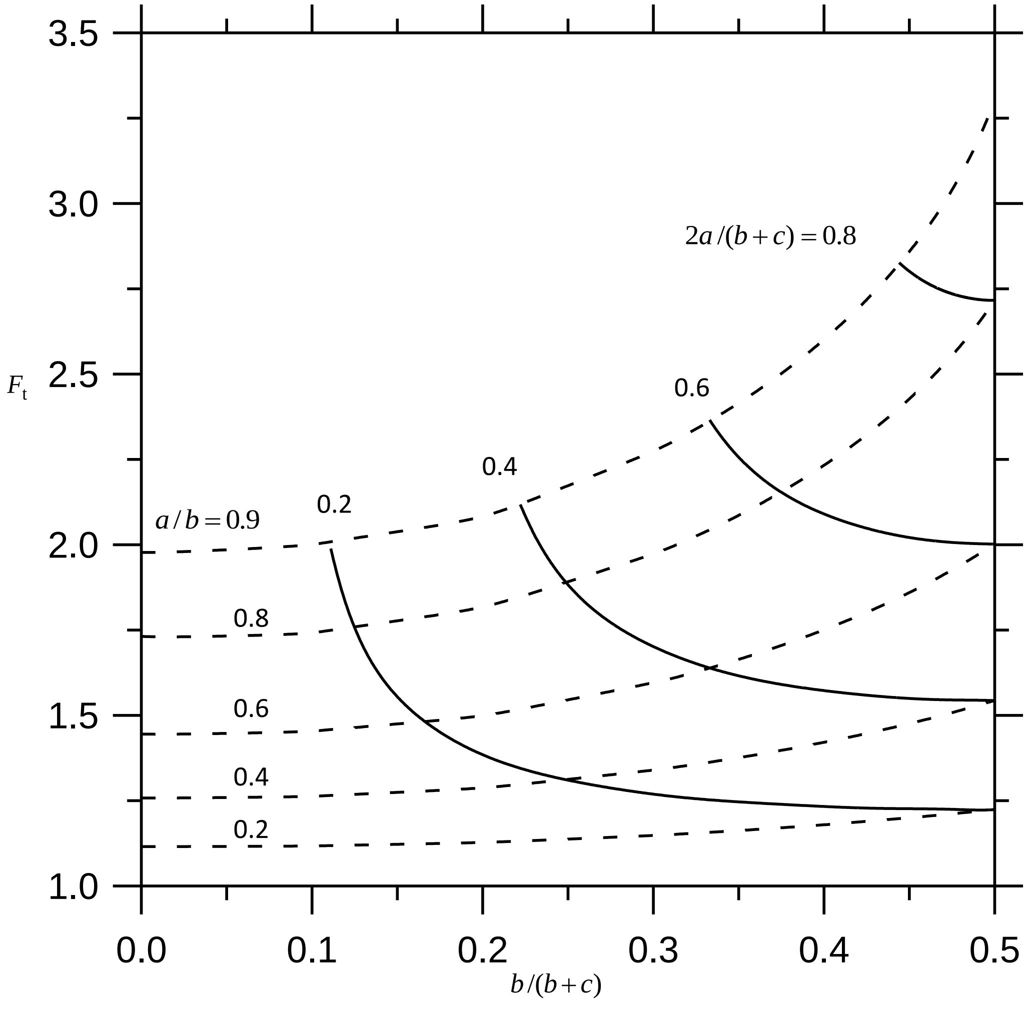

Fig. B1. Plots of the force coefficient F_t for the translation of a spherical particle with $\bar{\beta}a/\eta = 10$ parallel to two plane walls versus the ratio $b/(b+c)$ with a/b and $2a/(b+c)$ as parameters.

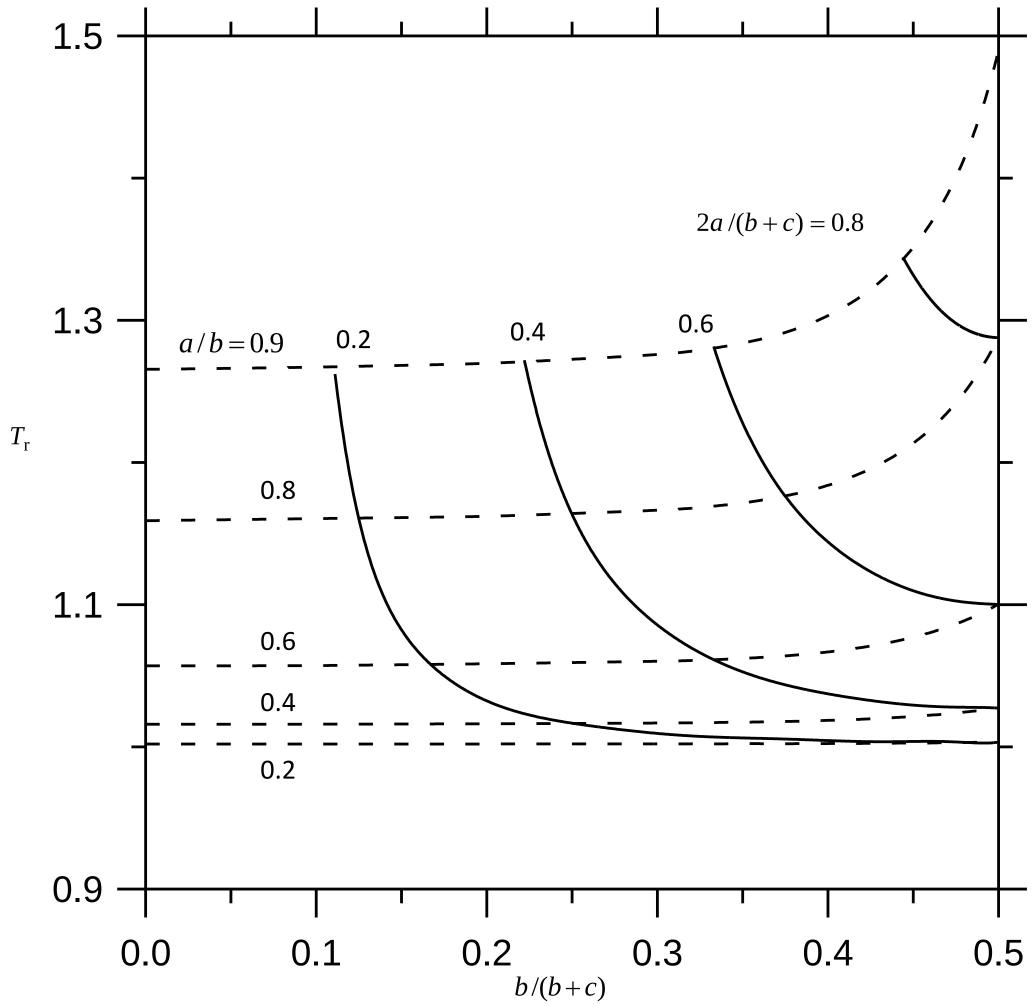

Fig. B2. Plots of the torque coefficient T_r for the rotation of a spherical particle with $\bar{\beta}a/\eta = 10$ parallel to two plane walls versus the ratio $b/(b+c)$ with a/b and $2a/(b+c)$ as parameters.

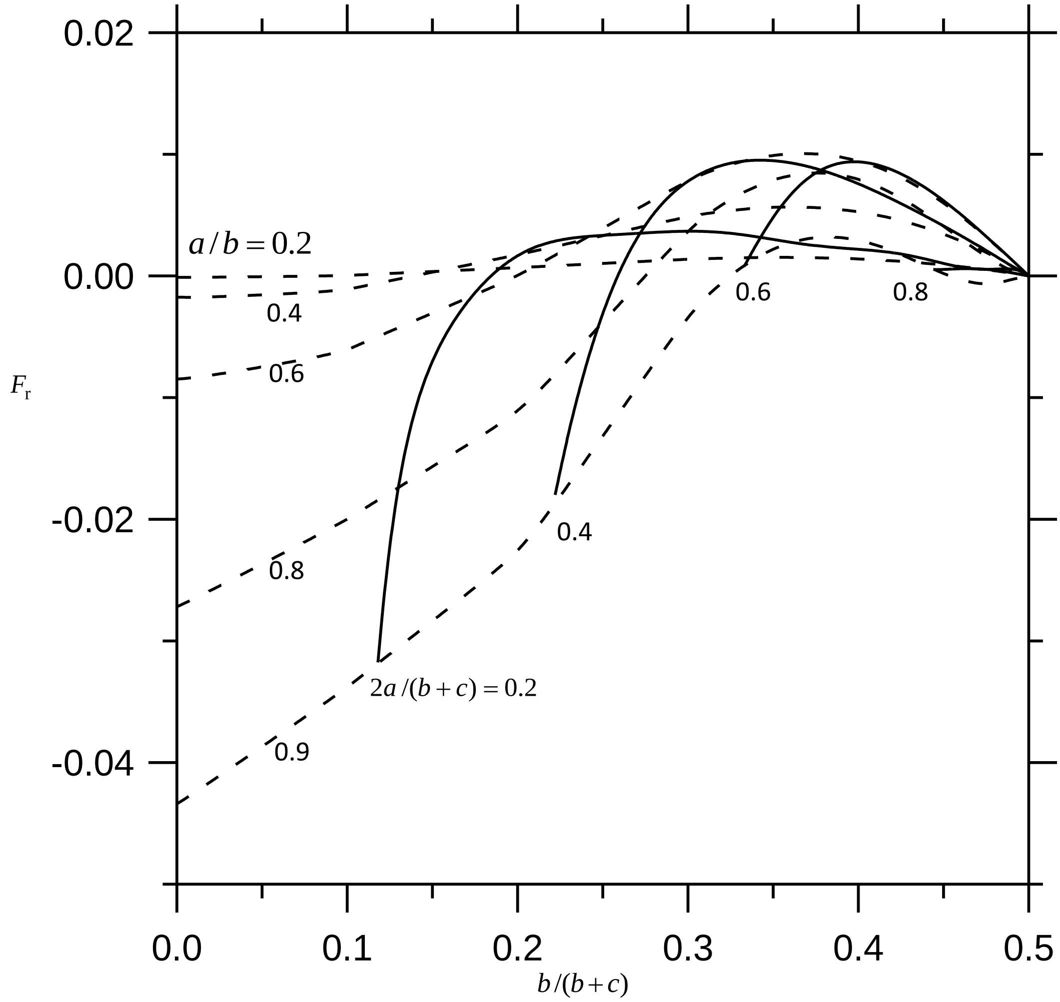

Fig. B3. Plots of the coupling coefficient $F_r = T_t(4/3)\bar{\beta}a/(\bar{\beta}a + 2\eta)$ for the motion of a spherical particle with $\bar{\beta}a/\eta = 10$ parallel to two plane walls versus the ratio $b/(b+c)$ with a/b and $2a/(b+c)$ as parameters.

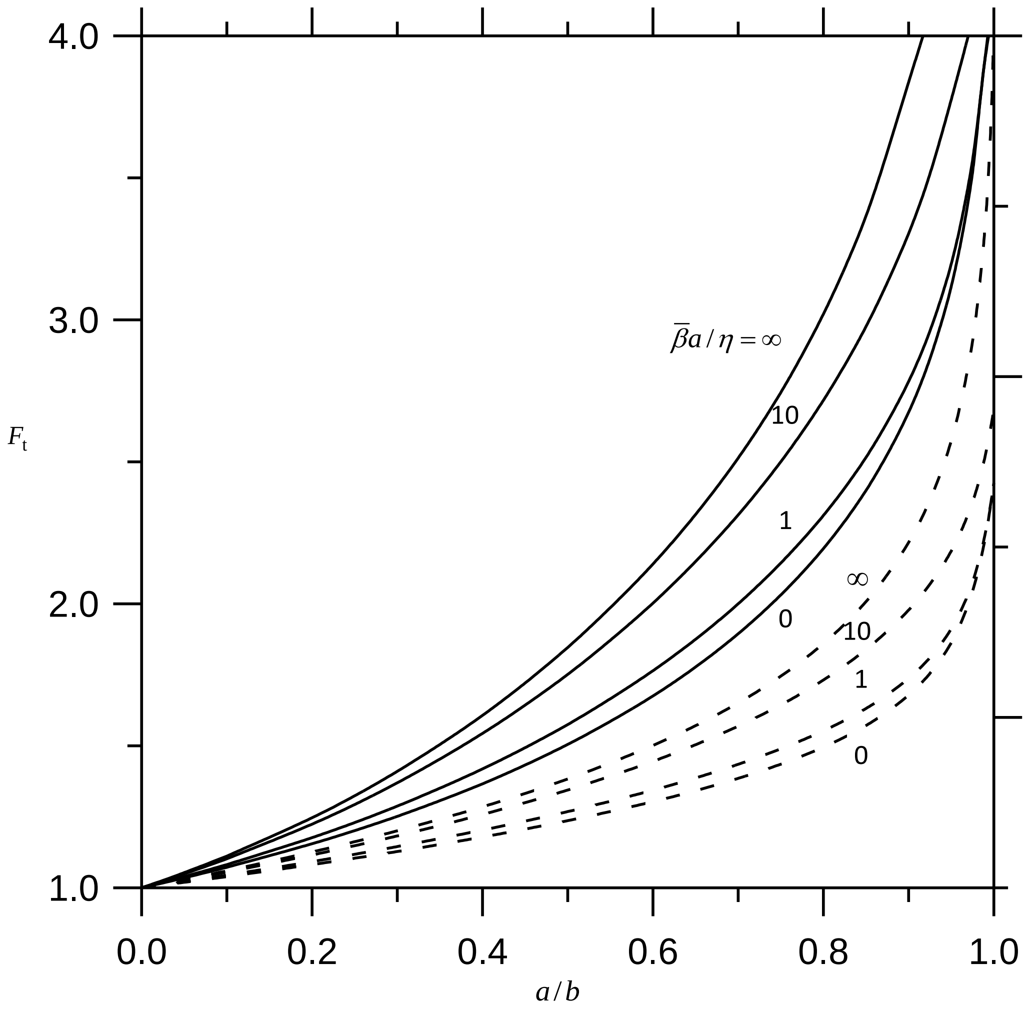

Fig. B4. Plots of the force coefficient F_t for the translation of a spherical particle with $\bar{\beta}a/\eta = 10$ on the midplane between two parallel plane walls (with $c = b$) versus the ratio a/b with $\bar{\beta}a/\eta$ as a parameter. The dashed curves are plotted for the translation of an identical particle parallel to a single plane wall for comparison.

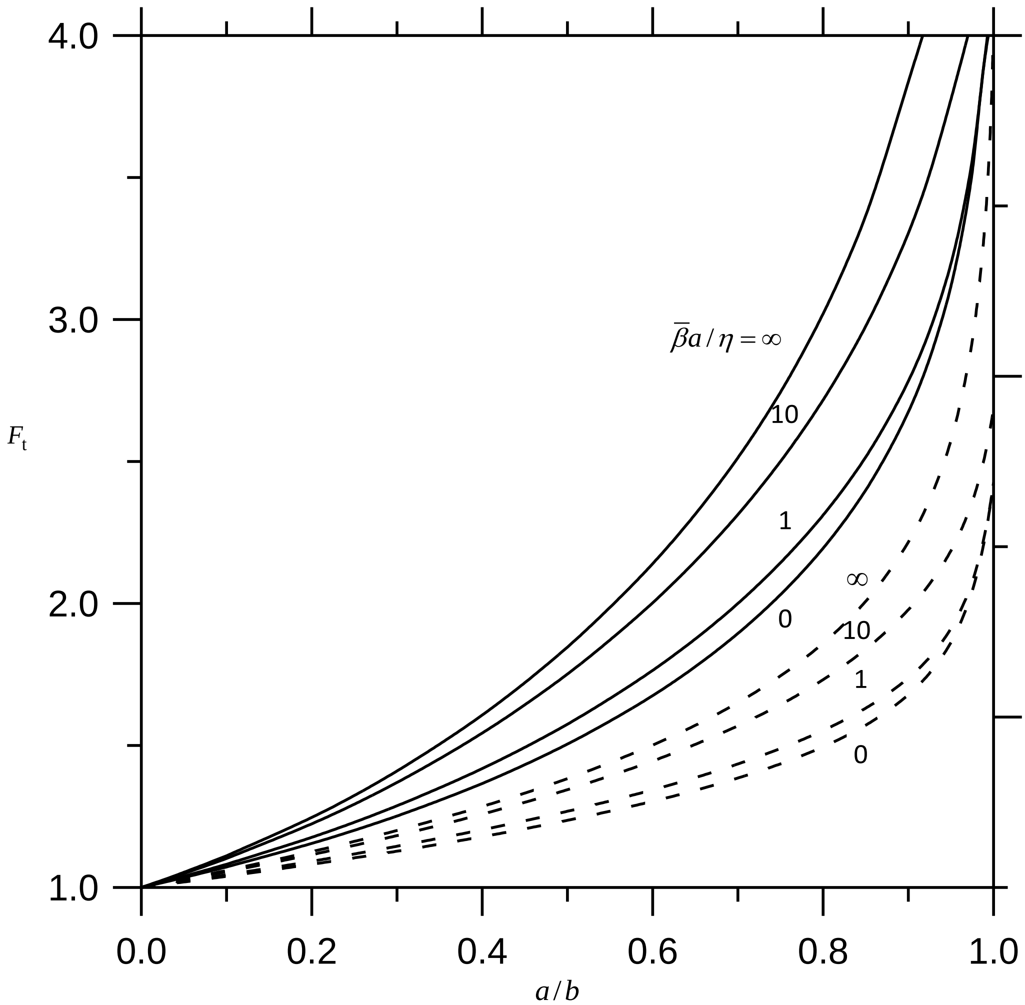

Fig. B5. Plots of the torque coefficient T_r for the rotation of a spherical particle with $\bar{\beta}a/\eta=10$ on the midplane between two parallel plane walls (with $c=b$) versus the ratio a/b with $\bar{\beta}a/\eta$ as a parameter. The dashed curves are plotted for the translation of an identical particle parallel to a single plane wall for comparison.

References

Basset, A. B., 1961. *A Treatise on Hydrodynamics*, Vol. 2, Dover, New York.

Chen, S. H. Keh, H. J., 1995a. Axisymmetric Motion of Two Spherical Particles with Slip Surfaces. *J. Colloid Interface Sci*., **171**, 63.

Davis, M. H., 1972. Collisions of Small Cloud Droplets: Gas Kinetic Effects. *J. Atoms. Sci*., **29**, 911.

Dean, W. R. O'Neill, M. E., 1963. A Slow Motion of Viscous Liquid Caused by the Rotation of a Solid Sphere. *Mathematica*, **10**, 13.

Ganatos, P., Weinbaum, S., Pfeffer, R., 1980. A strong interaction theory for the creeping motion of a sphere between plane parallel boundaries. Part 2. Parallel motion. *J. Fluid Mech.* **99**, 755.

Goldman, A. J., Cox, R. G., Brenner, H., 1967. Slow viscous motion of a sphere parallel to a plane wall- I. Motion through a quiescent fluid. *Chem. Engng. Sci.*, **22**, 637.

Hadamard, J. S., 1911. Mouvement permanent lent d'une sphere liquide et visqueuse dans un liquid visqueux. *Compt. Rend. Acad. Sci. (Paris)*, **152**, 1735.

Happel, J., Brenner, H., 1983. *Low Reynolds Number Hydrodynamics.* Nijhoff. The Hague, The Netherlands.

Hutchins, D. K., M. H. Harper, Felder, R. L., 1995. Slip Correction Measurements for Solid Spherical Particles by Modulated Dynamic Light Scattering. *Aerosol Sci. Technol*. **22**, 202.

Keh, H. J., Chang, J. H., 1998. Boundary Effects on the Creeping-Flow and Thermophoretic Motions of an Aerosol Particle in a Spherical Cavity. *Chem. Engng. Sci*., **53**, 2365.

Keh, H. J., Chen, P. Y., 2001. Slow motion of a droplet between two parallel plane walls. *Chem. Engng. Sci*., **56**, 6863.

Kennard, E. H., 1938. *Kinetic Theory of Gases*, McGraw-Hill, New York.

Kim, S. Karrila, S. J., 1991. *Microhydrodynamics*: *Principles and Selected Applications*. Butterworth-Heinemann, Boston, MA.

Loyalka, S. K., 1990. Slip and Jump Coefficients for Rarefied Gas Flows: Variational Results for Lennard-Jones and $n(r)$-6 Potentials. *Physica A*, **163**, 813.

O'Brien, V., 1968. Form factors for deformed spheroids in Stokes flow. *AIChE J* **14**, 870.

O'Neill, M. E., 1964. A slow motion of viscous liquid caused by a slowly moving solid sphere. *Mathematika*, **11**, 67.

Reed, L. D. Morrision, F. A., 1974. Particle Interactions in Viscous Flow at Small Values of Knudsen Number. *J*. *Aerosol Sci*., **5**, 175.

Rybczynski, W., 1911. Uber die fortschreitende bewegung einer flussigen kugel in einem zahen medium. *Bull*. *Acad*. *Sci*. *Cracovie Ser*. *A*, **1**, 40.

Stokes, G. G., 1851. On the Effect of The Internal Friction of Fluid on Pendulums. *Trans*. *Camb*. *Phil*. *Soc*., **9**, 8.

Talbot, L., Cheng, R. K., Schefer, R. W., Willis, D. R., 1980. Thermophoresis of Particles in Heated Boundary Layer. *J. Fluid Mech.*, **101**, 737.

Ying, R., Peters, M. H., 1991. Interparticle and Particle-Surface Gas Dynamic Interactions. *Aerosol Sci*. *Technol*., **14**, 418.

Appendix C. Analysis of the phoresismotions of a spherical particle parallel to one or two plane walls by a method of reflections

C1. Analysis of the diffusiophoresis of a spherical particle parallel to one or two plane walls by a method of reflections

In this section, I analyze the quasisteady diffusiophoretic motion of a colloidal sphere either parallel to an infinite flat wall ($c \to \infty$) or on the median plane between two parallel plates ($c = b$), as shown in Figure 2.1, by a method of reflections. The effect of the walls on the translational velocity U and angular velocity Ω of the particle is sought in expansions of λ, which equals a/b, the ratio of the particle radius to the distance between the wall and the center of the particle.

C1.1. *Motion parallel to an infinite plane wall*

For the problem of diffusiophoretic motion of a spherical particle parallel to an impermeable plane wall, the governing equations [2.1] and [2.13] must be solved by satisfying the boundary conditions [2.2], [2.5], [2.6], and [2.14]-[2.16] with $c \to \infty$. The method-of-reflection solution consists of the following series, whose terms depend on increasing powers of λ:

$$C = C_0 + E_\infty x + C_{\mathrm{p}}^{(1)} + C_{\mathrm{w}}^{(1)} + C_{\mathrm{p}}^{(2)} + C_{\mathrm{w}}^{(2)} + \dots, \qquad \text{[C1-1a]}$$

$$\mathrm{v} = \mathrm{v}_{\mathrm{p}}^{(1)} + \mathrm{v}_{\mathrm{w}}^{(1)} + \mathrm{v}_{\mathrm{p}}^{(2)} + \mathrm{v}_{\mathrm{w}}^{(2)} + \dots, \qquad \text{[C1-1b]}$$

where subscripts p and w represent the reflections from particle and wall, respectively, and the superscript [*i*] denotes the *i*th reflection from that surface. In these series, all the expansion sets of the corresponding concentration and velocity fields for the fluid solution must satisfy Eqs. [2.1] and [2.13]. The advantage of this method is that it is necessary to consider boundary conditions associated with only one surface at a time.

According to Eq. [C1-1], the translational and angular velocities of the particle can also be expressed in the series form,

$$\mathrm{U} = U_0 \mathrm{e}_x + \mathrm{U}^{(1)} + \mathrm{U}^{(2)} + \ldots, \qquad \text{[C1-2a]}$$

$$\Omega = \Omega^{(1)} + \Omega^{(2)} + \ldots \quad . \qquad \text{[C1-2b]}$$

In these expressions, $U_0 = AE_\infty$ is the diffusiophoretic velocity of an identical particle suspended freely in the continuous phase far from the wall given by Eq. [1-2.2]; $\mathrm{U}^{(i)}$ and $\Omega^{(i)}$ are related to $\nabla C_\mathrm{w}^{(i)}$ and $\mathbf{v}_\mathrm{w}^{(i)}$ by (Keh and Luo, 1995)

$$\mathrm{U}^{(i)} = A[\nabla C_\mathrm{w}^{(i)}]_0 + [\mathrm{v}_\mathrm{w}^{(i)}]_0 + \frac{a^2}{6}[\nabla^2 \mathrm{v}_\mathrm{w}^{(i)}]_0 , \qquad \text{[C1-3a]}$$

$$\Omega^{(i)} = \frac{1}{2}[\nabla \times \mathrm{v}_\mathrm{w}^{(i)}]_0 , \qquad \text{[C1-3b]}$$

where the subscript 0 to variables inside brackets denotes evaluation at the position of the particle center.

The solution for the first reflected fields from the particle is

$$C_\mathrm{p}^{(1)} = GE_\infty a^3 r^{-2} \sin\theta \cos\phi, \qquad \text{[C1-4a]}$$

$$\mathrm{v}_\mathrm{p}^{(1)} = \frac{1}{2} U_0 a^3 r^{-3} (2\sin\theta\cos\phi\, \mathrm{e}_r - \cos\theta\cos\phi\, \mathrm{e}_\theta + \sin\phi\, \mathrm{e}_\phi) , \qquad \text{[C1-4b]}$$

where $G = (1/2 - \beta/a)(1+\beta/a)^{-1}$. Obviously, $-1 \le G \le 1/2$, with the upper and lower bounds occuring at the limits $\beta/a = 0$ and $\beta/a \to \infty$, respectively. The velocity distribution shown in Eq. [C1-4b] is identical to the irrotational flow surrounding a rigid sphere moving with velocity $U_0 \mathrm{e}_x$.

The boundary conditions for the *i*th reflected fields from the wall are derived from Eqs. [2.5], [2.6], [2.15], and [2.16],

$$z = -b: \qquad \frac{\partial C_\mathrm{w}^{(i)}}{\partial z} = -\frac{\partial C_\mathrm{p}^{(i)}}{\partial z} , \qquad \text{[C1-5a]}$$

$$\mathrm{v}_\mathrm{w}^{(i)} = -\mathrm{v}_\mathrm{p}^{(i)} ; \qquad \text{[C1-5b]}$$

$$r \to \infty\,, \quad z > -b: \qquad C_{\mathrm{w}}^{(i)} \to 0\,, \qquad \text{[C1-5c]}$$

$$\mathrm{v}_{\mathrm{w}}^{(i)} \to 0\,. \qquad \text{[C1-5d]}$$

The solution of $C_{\mathrm{w}}^{(1)}$ is obtained by applying complex Fourier transforms on x and y in Eqs. [2.1] and [C1-5a, c], with the result

$$C_{\mathrm{w}}^{(1)} = G E_{\infty} a^3 x [x^2 + y^2 + (z+2b)^2]^{-3/2}\,. \qquad \text{[C1-6a]}$$

This reflected concentration field may be interpreted as arising from the reflection of the imposed field $E_{\infty}\mathrm{e}_x$ from a fictitious particle identical to the actual particle, its location being at the mirror-image position of the actual particle with respect to the plane $z = -b$ (i.e. at $x = 0, y = 0, z = -2b$). The solution for $\mathrm{v}_{\mathrm{w}}^{(1)}$ can be found by fitting the boundary conditions [C1-5b, d] with the general solution to Eq. [C1-13] established by Faxen (Happel and Brenner, 1983, p. 323), which results in

$$\mathrm{v}_{\mathrm{w}}^{(1)} = \frac{U_0 a^3}{4\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{i(\hat{\alpha}x + \hat{\beta}y) - \kappa(z+2b)} \{-[2\kappa(z+b)+1]\, i\hat{\alpha}\, \mathrm{e}_z$$

$$-[2\kappa(z+b)-1](\frac{\hat{\alpha}^2}{\kappa}\mathrm{e}_x + \frac{\hat{\alpha}\hat{\beta}}{\kappa}\mathrm{e}_y)\}\, \mathrm{d}\hat{\alpha}\, \mathrm{d}\hat{\beta}\,, \qquad \text{[C1-6b]}$$

where $\kappa = (\hat{\alpha}^2 + \hat{\beta}^2)^{1/2}$ and $i = \sqrt{-1}$.

The contributions of $C_{\mathrm{w}}^{(1)}$ and $\mathrm{v}_{\mathrm{w}}^{(1)}$ to the translational and angular velocities of the particle are determined by using Eq. [C1-3],

$$\mathrm{U}_{\mathrm{s}}^{(1)} = A[\nabla C_{\mathrm{w}}^{(1)}]_{r=0} = \frac{1}{8} G \lambda^3 U_0\, \mathrm{e}_x\,, \qquad \text{[C1-7a]}$$

$$\mathrm{U}_{\mathrm{h}}^{(1)} = [\mathrm{v}_{\mathrm{w}}^{(1)} + \frac{a^2}{6}\nabla^2 \mathrm{v}_{\mathrm{w}}^{(1)}]_{r=0} = -\frac{1}{8}(\lambda^3 - \lambda^5) U_0\, \mathrm{e}_x\,, \qquad \text{[C1-7b]}$$

$$\mathrm{U}^{(1)} = \mathrm{U}_{\mathrm{s}}^{(1)} + \mathrm{U}_{\mathrm{h}}^{(1)} = \frac{1}{8}[-(1-G)\lambda^3 + \lambda^5] U_0\, \mathrm{e}_x\,, \qquad \text{[C1-7c]}$$

$$a\Omega^{(1)} = \frac{a}{2}[\nabla \times \mathrm{v}_{\mathrm{w}}^{(1)}]_{r=0} = -\frac{3}{16} U_0 \lambda^4\, \mathrm{e}_y\,. \qquad \text{[C1-7d]}$$

Equation [C1-7a] shows that the reflected concentration field from the impermeable wall can increase (if $G > 0$ or $\beta / a < 1/2$) or decrease (if $G < 0$ or $\beta / a > 1/2$) the velocity of the diffusiophoretic particle, while Eq. [C1-7b] indicates that the reflected velocity field is to decrease this velocity; the net effect of the reflected fields is expressed by Eq. [C1-7c], which can enhance or retard the movement of the particle, depending on the combination of the values of G (or β/a) and λ. When $G=0$ (or $\beta/a=1/2$), the reflected solute concentration field makes no contribution to the diffusiophoretic velocity. Equation [C1-7c] indicates that the wall correction to the translational velocity of the diffusiophoretic particle is $\mathrm{O}(\lambda^3)$, which is weaker than that obtained for the corresponding sedimentation problem, in which the leading boundary effect is $\mathrm{O}(\lambda)$. Note that the necessary condition for the wall enhancement on the diffusiophoretic motion to occur is a small value of β/a and a value of λ close to unity such that the relation $\lambda^5 > (1-G)\lambda^3$ is warranted.

Equation [C1-7d] shows that the diffusiophoretic sphere rotates about an axis which is perpendicular to the direction of applied gradient and parallel to the plane wall. The direction of rotation is opposite to that which would occur if the sphere were driven to move by a body force. Note that the angular velocity $\Omega^{(1)}$ in Eq. [C1-7d] does not depend on the parameter G (since $\mathrm{v}_\mathrm{w}^{(1)}$ is not a function of G]. Also, the wall-induced angular velocity of the diffusiophoretic particle is $\mathrm{O}(\lambda^4)$, which is the same in order as but different in its coefficient ($-3/16$ versus $3/32$) from that of a rigid sphere moving under a body-force field (Happel and Brenner, 1983, p. 327).

The solution for the second reflected fields from the particle is

$$C_\mathrm{p}^{(2)} = \frac{1}{8}E_\infty[G^2\lambda^3a^3r^{-2}\sin\theta\cos\phi + GH\lambda^4a^4r^{-3}\cos\theta\sin\theta\cos\phi + \mathrm{O}(\lambda^5a^5)], \tag{C1-8a}$$

$$\begin{aligned}\mathrm{v}_\mathrm{p}^{(2)} = \frac{1}{32}U_0[&2G\lambda^3a^3r^{-3}(2\sin\theta\cos\phi\,\mathrm{e}_r - \cos\theta\cos\phi\,\mathrm{e}_\theta + \sin\phi\,\mathrm{e}_\phi) \\ &+ 9(4G\frac{B}{A}+5)\lambda^4a^2r^{-2}\cos\theta\sin\theta\cos\phi\,\mathrm{e}_r \\ &- \frac{3}{16}\lambda^4a^2r^{-2}(\cos\phi\,\mathrm{e}_\theta - \cos\theta\sin\phi\,\mathrm{e}_\phi) + \mathrm{O}(\lambda^4a^4, \lambda^5a^3)].\end{aligned} \tag{C1-8b}$$

Here, $H = 3(1-2\beta/a)(3+4\beta/a)^{-1}$ and $B = -(5kT/6\eta)L^*K(1+2\beta/a)^{-1}$.

The boundary conditions for the second reflected fields from the wall are obtained by substituting the results of $C_\mathrm{p}^{(2)}$ and $\mathrm{v}_\mathrm{p}^{(2)}$ into Eq. [C1-5], with which Eqs. [C1-1] and [C1-13] can be solved as before to yield

$$[\nabla C_{\mathrm{w}}^{(2)}]_{r=0} = [\frac{1}{64} G^2 \lambda^6 + \mathrm{O}(\lambda^8)] E_\infty \, \mathrm{e}_x , \qquad \text{[C1-9a]}$$

$$[\mathrm{v}_{\mathrm{w}}^{(2)}]_{r=0} = \{-\frac{1}{256}[4G(1+9\frac{B}{A})+39]\lambda^6 + \mathrm{O}(\lambda^8)\} U_0 \, \mathrm{e}_x . \qquad \text{[C1-9b]}$$

The contribution of the second reflected fields to the translational and angular velocities of the particle is obtained by putting $C_{\mathrm{w}}^{(2)}$ and $\mathrm{v}_{\mathrm{w}}^{(2)}$ into Eq. [C1-3], which gives

$$\mathrm{U}^{(2)} = \{\frac{1}{256}[4G^2 - 4G(1+9\frac{B}{A}) - 39]\lambda^6 + \mathrm{O}(\lambda^8)\} U_0 \, \mathrm{e}_x , \qquad \text{[C1-10a]}$$

$$a\Omega^{(2)} = \{[\frac{3}{256} G(1+39\frac{B}{A}) - \frac{93}{512}]\lambda^7 + \mathrm{O}(\lambda^9)\} U_0 \, \mathrm{e}_y . \qquad \text{[C1-10b]}$$

The errors for $\mathrm{U}^{(2)}$ and $a\Omega^{(2)}$ are $\mathrm{O}(\lambda^8)$ and $\mathrm{O}(\lambda^9)$, respectively, because the $\mathrm{O}(\lambda^7)$ terms in the expansions of $\nabla C_{\mathrm{w}}^{(2)}$ and $\mathrm{v}_{\mathrm{w}}^{(2)}$ vanish at the position of the particle center.

Obviously, $\mathrm{U}^{(3)}$ and $a\Omega^{(3)}$ will be $\mathrm{O}(\lambda^9)$ and $\mathrm{O}(\lambda^{10})$, respectively.

With the substitution of Eqs. [C1-7c, d] and [C1-10] into Eq. [C1-2], the particle velocities can be expressed as $\mathrm{U} = U\mathrm{e}_x$ and $\Omega = \mathit{\Omega}\mathrm{e}_y$ with

$$U = U_0\{1 - \frac{1}{8}(1-G)\lambda^3 + \frac{1}{8}\lambda^5$$

$$+ \frac{1}{256}[4G^2 - 4(1+9\frac{B}{A})G - 39]\lambda^6 + \mathrm{O}(\lambda^8)\} , \qquad \text{[C1-11a]}$$

$$a\mathit{\Omega} = U_0\{-\frac{3}{16}\lambda^4 + [\frac{3}{256} G(1+39\frac{B}{A}) - \frac{93}{512}]\lambda^7 + O(\lambda^9)\} . \qquad \text{[C1-11b]}$$

The particle migrates along the imposed solute concentration gradient at a rate that can increase or decrease as the particle approaches the wall. Owing to the neglect of inertial effects, the wall does not deflect the direction of diffusiophoresis.

For the case that a linear solute concentration profile is prescribed on the plane wall which is consistent with the far-field distribution, namely, the boundary condition [2.5] is replaced by Eq. [2.7], the series expansions [C1-1] and [C1-2], the solutions of $C_{\mathrm{p}}^{(1)}$ and $\mathrm{v}_{\mathrm{p}}^{(1)}$ in Eq. [C1-4], and the boundary conditions for $C_{\mathrm{w}}^{(i)}$ and $\mathrm{v}_{\mathrm{w}}^{(i)}$ in Eqs. [C1-5b-d] are still valid, while Eq. [C1-5a] becomes

$$z = -b: \qquad C_{\mathrm{w}}^{(i)} = -C_{\mathrm{p}}^{(i)} . \qquad \text{[C1-12]}$$

With this change, it can be shown that the results of the reflected fields and of the particle velocities are also obtained from Eqs. [C1-6]-[C1-11] by replacing G by $-G$. Thus, contrary to the effect of an impermeable plane wall, the reflected solute concentration field from a parallel wall with the imposed far-field concentration gradient reduces the translational velocity of the particle if $G > 0$ or $\beta / a < 1/2$ and enhances this velocity if $G < 0$ or $\beta / a > 1/2$. When $G = 0$ or $\beta / a = 1/2$, the two types of plane wall will produce the same effects on the diffusiophoretic motion of the particle. Under the conditions that the values of β / a and λ are sufficiently large such that $\lambda^5 > (1+G)\lambda^3$, the net effect of a lateral plane wall prescribed with the far-field concentration distribution can enhance the diffusiophoretic migration of a particle.

C1.2. *Motion on the median plane between two parallel flat walls*

For the problem of diffusiophoretic motion of a sphere on the median plane between two impermeable parallel plates, the boundary conditions corresponding to governing equations [2.1] and [2.13] are given by Eqs. [2.2], [2.5], [2.6], and [2.14]-[2.16] with $c = b$. But, the angular velocity Ω of the particle vanishes now because of the symmetry. With $\lambda = a/b << 1$, the series expansions of the solute concentration, fluid velocity, and particle velocity given by Eqs. [C1-1], [C1-2a], and [C1-4] remain valid here. From Eqs. [2.5], [2.6], [2.15], and [2.16], the boundary conditions for $C_{\mathrm{w}}^{(i)}$ and $\mathrm{v}_{\mathrm{w}}^{(i)}$ are found to be

$$|z| = b: \qquad \frac{\partial C_{\mathrm{w}}^{(i)}}{\partial z} = -\frac{\partial C_{\mathrm{p}}^{(i)}}{\partial z}, \tag{C1-13a}$$

$$\mathrm{v}_{\mathrm{w}}^{(i)} = -\mathrm{v}_{\mathrm{p}}^{(i)}; \tag{C1-13b}$$

$$r \to \infty, \ |z| \le b: \qquad C_{\mathrm{w}}^{(i)} \to 0, \tag{C1-13c}$$

$$\mathrm{v}_{\mathrm{w}}^{(i)} \to 0. \tag{C1-13d}$$

The first wall-reflected fields can be solved by the same method as used for a single lateral plate in the previous subsection , with the results

$$C_{\mathrm{w}}^{(1)} = -\frac{G E_\infty a^3}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{i\alpha}{\kappa}\,\mathrm{e}^{i(\hat{\alpha}x+\hat{\beta}y)-\kappa b}\,\frac{\cosh(\kappa z)}{\sinh(\kappa b)}\,\mathrm{d}\,\hat{\alpha}\,\mathrm{d}\,\hat{\beta}\,, \qquad \text{[C1-14a]}$$

$$\mathrm{v}_{\mathrm{w}}^{(1)} = \frac{U_0 a^3}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{\sinh(2\kappa b)-2\kappa b}\,\mathrm{e}^{i(\hat{\alpha}x+\hat{\beta}y)}$$

$$\{[\sinh(\kappa z)-\kappa z\cosh(\kappa z)+g\sinh(\kappa z)]\,i\hat{\alpha}\mathrm{e}_z$$

$$+[\kappa z\sinh(\kappa z)-g\cosh(\kappa z)](\frac{\hat{\alpha}^2}{\kappa}\mathrm{e}_x+\frac{\hat{\alpha}\hat{\beta}}{\kappa}\mathrm{e}_y)\}\,\mathrm{d}\,\hat{\alpha}\,\mathrm{d}\,\hat{\beta}\,, \qquad \text{[C1-14b]}$$

where $\kappa = (\hat{\alpha}^2+\hat{\beta}^2)^{1/2}$ and $g = \kappa b - \mathrm{e}^{-\kappa b}\sinh(\kappa b)$. The contributions of $C_{\mathrm{w}}^{(1)}$ and $\mathrm{v}_{\mathrm{w}}^{(1)}$ to the particle velocity are determined using Eq. [C1-3a], which lead to a result similar to Eqs. [C1-7a-c],

$$\mathrm{U}_{\mathrm{s}}^{(1)} = d_1 G\lambda^3 U_0\,\mathrm{e}_x\,, \qquad \text{[C1-15a]}$$

$$\mathrm{U}_{\mathrm{h}}^{(1)} = -(d_2\lambda^3 - d_3\lambda^5)U_0\,\mathrm{e}_x\,, \qquad \text{[C1-15b]}$$

$$\mathrm{U}^{(1)} = \mathrm{U}_{\mathrm{s}}^{(1)} + \mathrm{U}_{\mathrm{h}}^{(1)} = [-(d_2 - d_1 G)\lambda^3 + d_3\lambda^5]U_0\,\mathrm{e}_x\,, \qquad \text{[C1-15c]}$$

where

$$d_1 = \int_0^\infty \frac{\rho^2}{\mathrm{e}^{2\rho}-1}\,\mathrm{d}\,\rho = 0.300514\,, \qquad \text{[C1-16a]}$$

$$d_2 = \frac{1}{2}\int_0^\infty \frac{\rho^2(\rho-\mathrm{e}^{-\rho}\sinh\rho)}{\sinh(2\rho)-2\rho}\,\mathrm{d}\,\rho = 0.417956\,, \qquad \text{[C1-16b]}$$

$$d_3 = \frac{1}{6}\int_0^\infty \frac{\rho^4}{\sinh(2\rho)-2\rho}\,\mathrm{d}\,\rho = 0.338324\,. \qquad \text{[C1-16c]}$$

Analogous to the previous case, the results of the second reflections can be obtained as

$$C_{\mathrm{p}}^{(2)} = E_\infty[d_1 G^2\lambda^3 a^3 r^{-2}\sin\theta\cos\phi + \mathrm{O}(\lambda^5 a^5)]\,, \qquad \text{[C1-17a]}$$

$$\mathrm{v}_{\mathrm{p}}^{(2)} = \frac{U_0}{2}[d_1 G\lambda^3 a^3 r^{-3}(2\sin\theta\cos\phi\,\mathrm{e}_r - \cos\theta\cos\phi\,\mathrm{e}_\theta + \sin\phi\,\mathrm{e}_\phi) + \mathrm{O}(\lambda^5 a^3)]\,,$$

[C1-17b]

$$[\nabla C_{\mathrm{w}}^{(2)}]_{r=0} = [d_1^2 G^2\lambda^6 + \mathrm{O}(\lambda^8)]E_\infty\,\mathrm{e}_x\,, \qquad \text{[C1-18a]}$$

$$[\mathrm{v}_{\mathrm{w}}^{(2)}]_{r=0} = [-d_1 d_2 G\lambda^6 + \mathrm{O}(\lambda^8)]U_0\,\mathrm{e}_x\,, \qquad \text{[C1-18b]}$$

and

$$\mathrm{U}^{(2)} = [-(d_1 d_2 G - d_1^2 G^2)\lambda^6 + \mathrm{O}(\lambda^8)]U_0\,\mathrm{e}_x\,. \qquad \text{[C1-19]}$$

Note that the $\lambda^4 a^2$ and $\lambda^4 a^4$ terms in the expressions for $C_{\mathrm{p}}^{(2)}$ and $\mathrm{v}_{\mathrm{p}}^{(2)}$ vanish. With the combination of Eqs. [C1-2a], [C1-15c], and [C1-19], the particle velocity can be expressed as $\mathrm{U} = U\mathrm{e}_x$ with

$$U = U_0[1 - (d_2 - d_1 G)\lambda^3 + d_3\lambda^5 - (d_1 d_2 G - d_1^2 G^2)\lambda^6 + \mathrm{O}(\lambda^8)] . \qquad \text{[C1-20]}$$

For the case that the particle is undergoing diffusiophoresis on the median plane between two parallel plates on which a linear solute concentration profile consistent with the far-field distribution is imposed, Eq. [2.5] should be replaced by Eq. [2.7]. In this case, Eqs. [C1-1], [C1-2a], [C1-4] and [C1-13b-d] are still applicable, while Eq. [C1-13a] becomes

$$|z| = b: \qquad C_{\mathrm{w}}^{(i)} = -C_{\mathrm{p}}^{(i)} . \qquad \text{[C1-21]}$$

With this change, it can be shown that the results of the reflected fields and of the particle velocity are also obtained from Eq. [C1-14]-[C1-20] by replacing G and d_1 by $-G$ and $\bar{d}_1$, respectively, where

$$\bar{d}_1 = \int_0^\infty \frac{\rho^2}{\mathrm{e}^{2\rho}+1}\,\mathrm{d}\rho = 0.225386 . \qquad \text{[C1-22]}$$

Comparing Eq. [C1-20] for the slit case with Eq. [C1-11a] for the case of a single parallel plane, one can find that the wall effects on the diffusiophoretic velocity of a particle in the two cases are qualitatively similar. However, the assumption that the result of the boundary effect for two walls can be obtained by simple addition of the single-wall effects generally gives a smaller correction to diffusiophoretic velocity, while for the corresponding sedimentation problem this approximation overestimates the wall correction.

C2. Analysis of the osmophoresis of a spherical vesicle parallel to plane walls by a method of reflections

In this section, I analyze the quasisteady osmophoretic motion of a spherical vesicle either parallel to an infinite flat wall ($c \to \infty$) or on the median plane between two parallel plates ($c = b$), as shown in Figure 3.1, by a method of reflections. The effect of the walls on the translational velocity U and angular velocity Ω of the vesicle is sought in expansions of λ, which equals a/b, the ratio of the vesicle radius to the distance between the wall and the center of the vesicle.

C2.1. *Motion parallel to an infinite plane wall*

For the problem of osmophoretic motion of a spherical vesicle parallel to an impermeable plane wall, the governing equations [3.1a] and [3.12] must be solved by satisfying the boundary conditions [3.2]-[3.4] and [3.13]-[3.15] with $c \to \infty$. The method-of-reflection solution consists of the following series, whose terms depend on increasing powers of λ:

$$C = C_0 - E_\infty x + C_\mathrm{p}^{(1)} + C_\mathrm{w}^{(1)} + C_\mathrm{p}^{(2)} + C_\mathrm{w}^{(2)} + \ldots, \qquad \text{[C2-1a]}$$

$$\mathrm{v} = \mathrm{v}_\mathrm{p}^{(1)} + \mathrm{v}_\mathrm{w}^{(1)} + \mathrm{v}_\mathrm{p}^{(2)} + \mathrm{v}_\mathrm{w}^{(2)} + \ldots, \qquad \text{[C2-1b]}$$

where subscripts w and p represent the reflections from wall and vesicle, respectively, and the superscript (i) denotes the ith reflection from that surface. In these series, all the expansion sets of the corresponding solute concentration and fluid velocity for the solution phase outside the vesicle must satisfy Eqs. [3.1a] and [3.12]. The advantage of this method is that it is necessary to consider boundary conditions associated with only one surface at a time.

According to Eq. [C2-1], the translational and angular velocities of the vesicle can also be expressed in the series form,

$$\mathrm{U} = U_0 \mathrm{e}_x + \mathrm{U}^{(1)} + \mathrm{U}^{(2)} + \ldots, \qquad \text{[C2-2a]}$$

$$\Omega = \Omega^{(1)} + \Omega^{(2)} + \ldots \ . \qquad \text{[C2-2b]}$$

In these expressions, $U_0 = AE_\infty$ is the osmophoretic velocity of an identical vesicle suspended freely in the continuous phase far from the wall given by Eq. [1-3.1]; $\mathrm{U}^{(i)}$ and $\Omega^{(i)}$ are related to $\nabla C_{\mathrm{w}}^{(i)}$ and $\mathrm{v}_{\mathrm{w}}^{(i)}$ by (Keh and Tu, 2000)

$$\mathrm{U}^{(i)} = -A[\nabla C_{\mathrm{w}}^{(i)}]_0 + [\mathrm{v}_{\mathrm{w}}^{(i)}]_0 + \frac{a^2}{6}[\nabla^2 \mathrm{v}_{\mathrm{w}}^{(i)}]_0 , \qquad \text{[C2-3a]}$$

$$\Omega^{(i)} = \frac{1}{2}[\nabla \times \mathrm{v}_{\mathrm{w}}^{(i)}]_0 , \qquad \text{[C2-3b]}$$

where the subscript 0 to variables inside brackets denotes evaluation at the position of the vesicle center.

The solution for the first reflected fields from the vesicle is

$$C_{\mathrm{p}}^{(1)} = -GE_\infty a^3 r^{-2} \sin\theta \cos\phi, \qquad \text{[C2-4a]}$$

$$\mathrm{v}_{\mathrm{p}}^{(1)} = -U_0 a^3 r^{-3}(2\sin\theta\cos\phi\, \mathrm{e}_r - \cos\theta\cos\phi\, \mathrm{e}_\theta + \sin\phi\, \mathrm{e}_\phi) , \qquad \text{[C2-4b]}$$

where $G = (1+\bar{\kappa}-\kappa)(2+2\bar{\kappa}+\kappa)^{-1}$. Obviously, $-1 \le G \le 1/2$, with the upper and lower bounds occuring at the limits $\kappa << 1+\bar{\kappa}$ and $\kappa >> 2(1+\bar{\kappa})$, respectively. The velocity distribution shown in Eq. [C2-4b] is identical to the irrotational flow surrounding a rigid sphere moving with velocity $-2U_0 \mathrm{e}_x$.

The boundary conditions for the *i*th reflected fields from the wall are derived from Eqs. [3.3], [3.4], [3.14], and [3.15],

$$z = -b: \qquad \frac{\partial C_{\mathrm{w}}^{(i)}}{\partial z} = -\frac{\partial C_{\mathrm{p}}^{(i)}}{\partial z} , \qquad \text{[C2-5a]}$$

$$\mathrm{v}_{\mathrm{w}}^{(i)} = -\mathrm{v}_{\mathrm{p}}^{(i)} ; \qquad \text{[C2-5b]}$$

$$r \to \infty , \quad z > -b: \qquad C_{\mathrm{w}}^{(i)} \to 0 , \qquad \text{[C2-5c]}$$

$$\mathrm{v}_{\mathrm{w}}^{(i)} \to 0 . \qquad \text{[C2-5d]}$$

The solution of $C_{\mathrm{w}}^{(1)}$ is obtained by applying complex Fourier transforms on *x* and *y* in Eqs. [3.1a] and [C2-5a, c] (taking $i = 1$), with the result

$$C_{\mathrm{w}}^{(1)} = -GE_\infty a^3 x[x^2 + y^2 + (z+2b)^2]^{-3/2} . \qquad \text{[C2-6a]}$$

This reflected concentration field may be interpreted as arising from the reflection of the imposed field $-E_\infty \mathrm{e}_x$ from a fictitious vesicle identical to the actual vesicle, its location being at the mirror-image position of the actual vesicle with respect to the plane $z = -b$ (i.e. at $x = 0, y = 0, z = -2b$). The solution for $\mathrm{v}_\mathrm{w}^{(1)}$ can be found by fitting the boundary conditions [C2-5b, d] with the general solution to Eq. [3.12] established by Faxen (Happel and Brenner, 1983, p. 323), which results in

$$\mathrm{v}_\mathrm{w}^{(1)} = -\frac{U_0 a^3}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i(\alpha x+\beta y)-\gamma(z+2b)}\{-[2\gamma(z+b)+1] i\alpha\, \mathrm{e}_z$$

$$-[2(z+b)-\frac{1}{\gamma}](\alpha^2\mathrm{e}_x+\alpha\beta\mathrm{e}_y)\}\,\mathrm{d}\alpha\,\mathrm{d}\beta\,, \qquad \text{[C2-6b]}$$

where $\gamma = (\alpha^2+\beta^2)^{1/2}$, and $i = \sqrt{-1}$.

The contributions of $C_\mathrm{w}^{(1)}$ and $\mathrm{v}_\mathrm{w}^{(1)}$ to the translational and angular velocities of the vesicle are determined by using Eq. [C2-3],

$$\mathrm{U}_\mathrm{s}^{(1)} = -A[\nabla C_\mathrm{w}^{(1)}]_{r=0} = \frac{1}{8}G\lambda^3 U_0 \mathrm{e}_x\,, \qquad \text{[C2-7a]}$$

$$\mathrm{U}_\mathrm{h}^{(1)} = [\mathrm{v}_\mathrm{w}^{(1)} + \frac{a^2}{6}\nabla^2\mathrm{v}_\mathrm{w}^{(1)}]_{r=0} = \frac{1}{4}(\lambda^3-\lambda^5)U_0\mathrm{e}_x\,, \qquad \text{[C2-7b]}$$

$$\mathrm{U}^{(1)} = \mathrm{U}_\mathrm{s}^{(1)} + \mathrm{U}_\mathrm{h}^{(1)} = [\frac{1}{8}(2+G)\lambda^3 - \frac{1}{4}\lambda^5]U_0\mathrm{e}_x\,, \qquad \text{[C2-7c]}$$

$$a\Omega^{(1)} = \frac{a}{2}[\nabla\times\mathrm{v}_\mathrm{w}^{(1)}]_{r=0} = \frac{3}{8}\lambda^4 U_0\mathrm{e}_y\,. \qquad \text{[C2-7d]}$$

Equation [C2-7a] shows that the reflected solute concentration field from the impermeable wall can increase (if $G > 0$ or $\kappa < 1+\bar{\kappa}$) or decrease (if $G < 0$ or $\kappa > 1+\bar{\kappa}$) the translational velocity of the osmophoretic vesicle, while Eq. [C2-7b] indicates that the reflected velocity field is to *increase* this velocity; the net effect of the reflected fields is expressed by Eq. [C2-7c], which can enhance or retard the movement of the vesicle, depending on the combination of the values of G (or κ and $\bar{\kappa}$) and λ. When $G = 0$ (or $\kappa = 1+\bar{\kappa}$), the reflected concentration field makes no contribution to the osmophoretic velocity. Equation [C2-7c] indicates that the wall correction to the translational velocity of the osmophoretic vesicle is $\mathrm{O}(\lambda^3)$, which is weaker than that obtained for the corresponding sedimentation problem, in which the leading boundary effect is $\mathrm{O}(\lambda)$. Note that the necessary condition for the wall retardation on the osmophoretic motion to occur is $\kappa >> 1+\bar{\kappa}$ and a value of λ close to unity such that the relation $\lambda^5 > (1+G/2)\lambda^3$ is warranted.

Equation [C2-7d] shows that the osmophoretic sphere rotates about an axis which is perpendicular to the direction of the applied solute gradient and parallel to the plane wall. The direction of rotation is the same as that which would occur if a rigid sphere is driven to move parallel to the plane wall by a body force. Note that the angular velocity $\Omega^{(1)}$ in Eq. [C2-7d] does not depend on the parameter G (since $\mathrm{v}_\mathrm{w}^{(1)}$ is not a function of G). Also, the wall-induced angular velocity of the osmophoretic vesicle is $\mathrm{O}(\lambda^4)$, which is the same in order as but different in its coefficient ($3/8$ versus $3/32$) from that of a rigid sphere moving under a body-force field (Happel and Brenner, 1983, p. 327).

The solution for the second reflected fields from the vesicle is

$$C_\mathrm{p}^{(2)} = -\frac{1}{8}E_\infty[G^2\lambda^3 a^3 r^{-2}\sin\theta\cos\phi + 3GH\lambda^4 a^4 r^{-3}\cos\theta\sin\theta\cos\phi + \mathrm{O}(\lambda^5 a^5)], \qquad \text{[C2-8a]}$$

$$\begin{aligned}\mathrm{v}_\mathrm{p}^{(2)} = -\frac{1}{16}U_0[&2G\lambda^3 a^3 r^{-3}(2\sin\theta\cos\phi\,\mathrm{e}_r - \cos\theta\cos\phi\,\mathrm{e}_\theta + \sin\phi\,\mathrm{e}_\phi) \\ &-3(2G\frac{B}{A} - 15)\lambda^4 a^2 r^{-2}\cos\theta\sin\theta\cos\phi\,\mathrm{e}_r \\ &-6\lambda^4 a^2 r^{-2}(\cos\phi\,\mathrm{e}_\theta - \cos\theta\sin\phi\,\mathrm{e}_\phi) + \mathrm{O}(\lambda^4 a^4, \lambda^5 a^3)].\end{aligned} \qquad \text{[C2-8b]}$$

Here, $H = (2+\bar{\kappa}-\kappa)(6+3\bar{\kappa}+2\kappa)^{-1}$, $B = 5aL_\mathrm{p}RT(6+3\bar{\kappa}+2\kappa)^{-1}$.

The boundary conditions for the second reflected fields from the wall are obtained by substituting the results of $C_\mathrm{p}^{(2)}$ and $\mathrm{v}_\mathrm{p}^{(2)}$ into Eq. [C2-5], with which Eqs. [3.1a] and [3.12] can be solved as before to yield

$$[\nabla C_\mathrm{w}^{(2)}]_{r=0} = -[\frac{1}{64}G^2\lambda^6 + \mathrm{O}(\lambda^8)]E_\infty \mathrm{e}_x, \qquad \text{[C2-9a]}$$

$$[\mathrm{v}_\mathrm{w}^{(2)}]_{r=0} = \{\frac{1}{128}[39 + 2(2-3\frac{B}{A})G]\lambda^6 + \mathrm{O}(\lambda^8)\}U_0\mathrm{e}_x. \qquad \text{[C2-9b]}$$

The contribution of the second reflected fields to the translational and angular velocities of the vesicle is obtained by combining Eqs. [C2-3] and [C2-9], which gives

$$\mathrm{U}^{(2)} = \{\frac{1}{128}[39 + 2(2-3\frac{B}{A})G + 2G^2]\lambda^6 + \mathrm{O}(\lambda^8)\}U_0\mathrm{e}_x, \qquad \text{[C2-10a]}$$

$$a\Omega^{(2)} = \{\frac{3}{256}[19 + 4(1-8\frac{B}{A}G)]\lambda^7 + \mathrm{O}(\lambda^9)\}U_0\,\mathrm{e}_y. \qquad \text{[C2-10b]}$$

The errors for $\mathrm{U}^{(2)}$ and $a\Omega^{(2)}$ are $\mathrm{O}(\lambda^8)$ and $\mathrm{O}(\lambda^9)$, respectively, because the $\mathrm{O}(\lambda^7)$ terms in the expansions of $\nabla C_{\mathrm{w}}^{(2)}$ and $\mathrm{v}_{\mathrm{w}}^{(2)}$ vanish at the position of the vesicle center.

Obviously, $\mathrm{U}^{(3)}$ and $a\Omega^{(3)}$ will be $\mathrm{O}(\lambda^9)$ and $\mathrm{O}(\lambda^{10})$, respectively. With the substitution of Eqs. [C2-7c,d] and [C2-10] into Eq. [C2-2], the vesicle velocities can be expressed as $\mathbf{U} = U\mathbf{e}_x$ and $\Omega = \Omega \mathrm{e}_y$ with

$$U = U_0\{1+\frac{1}{8}(2+G)\lambda^3 - \frac{1}{4}\lambda^5 + \frac{1}{128}[39+2(2-3\frac{B}{A})G+2G^2]\lambda^6 + \mathrm{O}(\lambda^8)\}\,,$$

[C2-11a]

$$a\Omega = U_0\{\frac{3}{8}\lambda^4 + \frac{3}{256}[19+4(1-8\frac{B}{A})G]\lambda^7 + O(\lambda^9)\}\,. \qquad \text{[C2-11b]}$$

The vesicle migrates along the imposed concentration gradient at a rate that can increase or decrease as the vesicle approaches the wall. Owing to the neglect of inertial effects, the wall does not deflect the direction of osmophoresis.

For the case that a linear concentration profile is prescribed on the plane wall which is consistent with the far-field solute distribution, namely, the boundary condition Eq. [3.3] is replaced by Eq. [3.5], the series expansions [C2-1] and [C2-2], the solution of $C_{\mathrm{p}}^{(1)}$ and $\mathrm{v}_{\mathrm{p}}^{(1)}$ in Eq. [C2-4], and the boundary conditions for $C_{\mathrm{w}}^{(i)}$ and $\mathrm{v}_{\mathrm{w}}^{(i)}$ in Eqs. [C2-5b-d] are still valid, while Eq. [C2-5a] becomes

$$z = -b: \qquad C_{\mathrm{w}}^{(i)} = -C_{\mathrm{p}}^{(i)}\,. \qquad \text{[C2-12]}$$

With this change, it can be shown that the results of the following reflected fields and of the vesicle velocities are also obtained from Eqs. [C2-6]-[C2-11] by replacing G by $-G$. Thus, contrary to the effect of an impermeable plane wall, the reflected concentration field from a parallel wall with the imposed far-field concentration gradient reduces the translational velocity of the vesicle if $G>0$ or $\kappa < 1+\bar{\kappa}$ and enhances this velocity if $G<0$ or $\kappa > 1+\bar{\kappa}$. When $G=0$ or $\kappa = 1+\bar{\kappa}$, the two types of plane wall will produce the same effects (with no contribution from the reflected solute concentration field) on the osmophoretic motion of the vesicle. Under the condition that $\kappa << 1+\bar{\kappa}$ and the value of λ is sufficiently large such that $\lambda^5 > (1-G/2)\lambda^3$, the net effect of a lateral plane wall prescribed with the far-field solute concentration distribution can retard the osmophoretic migration of a vesicle.

C2.2. *Motion on the median plane between two parallel flat walls*

For the problem of osmophoretic motion of a spherical vesicle on the median plane between two impermeable parallel plates, the boundary conditions corresponding to governing equations [3.1a] and [3.12] are given by Eqs. [3.2]-[3.4] and [3.13]-[3.15] with $c = b$. But, the angular velocity Ω of the vesicle vanishes now because of the symmetry. With $\lambda = a/b << 1$, the series expansions of the solute concentration, fluid velocity, and vesicle velocity given by Eqs. [C2-1], [C2-2a], and [C2-4] remain valid here. From Eqs. [3.3], [3.4], [3.14], and [3.15], the boundary conditions for $C_{\mathrm{w}}^{(i)}$ and $\mathrm{v}_{\mathrm{w}}^{(i)}$ are found to be

$$|z| = b: \qquad \frac{\partial C_{\mathrm{w}}^{(i)}}{\partial z} = -\frac{\partial C_{\mathrm{p}}^{(i)}}{\partial z}, \tag{C2-13a}$$

$$\mathrm{v}_{\mathrm{w}}^{(i)} = -\mathrm{v}_{\mathrm{p}}^{(i)}; \tag{C2-13b}$$

$$r \to \infty, \quad |z| \le b: \qquad C_{\mathrm{w}}^{(i)} \to 0, \tag{C2-13c}$$

$$\mathrm{v}_{\mathrm{w}}^{(i)} \to 0. \tag{C2-13d}$$

The first wall-reflected fields can be solved by the same method as used for a single lateral plate in the previous subsection , with the results

$$C_{\mathrm{w}}^{(1)} = \frac{GE_\infty a^3}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{i\alpha}{\gamma} e^{i(\alpha x + \beta y) - \gamma b} \frac{\cosh(\gamma z)}{\sinh(\gamma b)} \,\mathrm{d}\alpha\,\mathrm{d}\beta, \tag{C2-14a}$$

$$\mathrm{v}_{\mathrm{w}}^{(1)} = -\frac{U_0 a^3}{\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{1}{\sinh(2\gamma b) - 2\gamma b} e^{i(\alpha x + \beta y)} \{[\sinh(\gamma z) - \gamma z \cosh(\gamma z) + g \sinh(\gamma z)] i\alpha \mathrm{e}_z$$
$$+ [z \sinh(\gamma z) - \frac{g}{\gamma}\cosh(\gamma z)](\alpha^2 \mathrm{e}_x + \alpha\beta \mathrm{e}_y)\} \,\mathrm{d}\alpha\,\mathrm{d}\beta, \tag{C2-14b}$$

where $\gamma = (\alpha^2 + \beta^2)^{1/2}$ and $g = \gamma b - \mathrm{e}^{-\gamma b}\sinh(\gamma b)$. The contributions of $C_{\mathrm{w}}^{(1)}$ and $\mathrm{v}_{\mathrm{w}}^{(1)}$ to the vesicle velocity are determined using Eq. [C2-3a], which lead to a result similar to Eqs. [C2-7a-c],

$$\mathrm{U}_{\mathrm{s}}^{(1)} = d_1 G \lambda^3 U_0 \,\mathrm{e}_x, \tag{C2-15a}$$

$$\mathrm{U}_{\mathrm{h}}^{(1)} = (d_2 \lambda^3 - d_3 \lambda^5) U_0 \,\mathrm{e}_x, \tag{C2-15b}$$

$$\mathrm{U}^{(1)} = \mathrm{U}_{\mathrm{s}}^{(1)} + \mathrm{U}_{\mathrm{h}}^{(1)} = [(d_2 + d_1 G)\lambda^3 - d_3 \lambda^5] U_0 \mathrm{e}_x \,, \qquad \text{[C2-15c]}$$

where

$$d_1 = \int_0^\infty \frac{\rho^2}{\mathrm{e}^{2\rho} - 1} \mathrm{d}\rho = 0.300514 \,, \qquad \text{[C2-16a]}$$

$$d_2 = \int_0^\infty \frac{\rho^2 (\rho - \mathrm{e}^{-\rho} \sinh\rho)}{\sinh(2\rho) - 2\rho} \mathrm{d}\rho = 0.835912 \,, \qquad \text{[C2-16b]}$$

$$d_3 = \frac{1}{3} \int_0^\infty \frac{\rho^4}{\sinh(2\rho) - 2\rho} \mathrm{d}\rho = 0.676648 \,. \qquad \text{[C2-16c]}$$

Analogous to the previous case, the results of the second reflections can be obtained as

$$C_{\mathrm{p}}^{(2)} = -E_\infty [d_1 G^2 \lambda^3 a^3 r^{-2} \sin\theta \cos\phi + \mathrm{O}(\lambda^5 a^5)] \,, \qquad \text{[C2-17a]}$$

$$\mathrm{v}_{\mathrm{p}}^{(2)} = U_0 [-d_1 G \lambda^3 a^3 r^{-3} (2 \sin\theta \cos\phi \, \mathrm{e}_r - \cos\theta \cos\phi \, \mathrm{e}_\theta + \sin\phi \, \mathrm{e}_\phi) + \mathrm{O}(\lambda^5 a^3)] \,,$$

$$\text{[C2-17b]}$$

$$[\nabla C_{\mathrm{w}}^{(2)}]_{r=0} = -[d_1^2 G^2 \lambda^6 + \mathrm{O}(\lambda^8)] E_\infty \mathrm{e}_x \,, \qquad \text{[C2-18a]}$$

$$[\mathrm{v}_{\mathrm{w}}^{(2)}]_{r=0} = [d_1 d_2 G \lambda^6 + \mathrm{O}(\lambda^8)] U_0 \mathrm{e}_x \,, \qquad \text{[C2-18b]}$$

and

$$\mathrm{U}^{(2)} = [(d_1 d_2 G + d_1^2 G^2)\lambda^6 + \mathrm{O}(\lambda^8)] U_0 \mathrm{e}_x \,. \qquad \text{[C2-19]}$$

Note that the $\lambda^4 a^2$ and $\lambda^4 a^4$ terms in the expressions for $C_{\mathrm{p}}^{(2)}$ and $\mathrm{v}_{\mathrm{p}}^{(2)}$ vanish. With the combination of Eqs. [C2-2a], [C2-15c], and [C2-19], the vesicle velocity can be expressed as $\mathrm{U} = U \mathrm{e}_x$ with

$$U = U_0 [1 + (d_2 + d_1 G)\lambda^3 - d_3 \lambda^5 + (d_1 d_2 G + d_1^2 G^2)\lambda^6 + \mathrm{O}(\lambda^8)] \,. \qquad \text{[C2-20]}$$

For the case that the vesicle is undergoing osmophoresis on the median plane between two parallel plates on which a linear concentration profile consistent with the far-field solute distribution is imposed, the boundary condition given by Eq. [3.3] should be replaced by Eq. [3.5]. In this case, Eqs. [C2-1], [C2-2a], [C2-4] and [C2-13b-d] are still applicable, while Eq. [C2-13a] becomes

$$|z| = b : \qquad C_{\mathrm{w}}^{(i)} = -C_{\mathrm{p}}^{(i)} \,. \qquad \text{[C2-21]}$$

With this change, it can be shown that the results of the reflected fields and of the vesicle velocity are also obtained from Eq. [C2-14]-[C2-20] by replacing G and d_1 by $-G$ and $\bar{d}_1$, respectively, where

$$\bar{d}_1 = \int_0^\infty \frac{\rho^2}{e^{2\rho}+1} \mathrm{d}\rho = 0.225386 . \qquad [C2-22]$$

Comparing Eq. [C2-20] for the slit case with Eq. [C2-11a] for the case of a single parallel plane, one can find that the wall effects on the osmophoretic velocity of a vesicle in the two cases are qualitatively similar. However, the assumption that the result of the boundary effect for two walls can be obtained by simple addition of the single-wall effects generally gives a smaller correction to the osmophoretic velocity, while for the corresponding sedimentation problem this approximation overestimates the wall correction.

C3. Analysis of the thermocapillary migration of a droplet parallel to plane walls by a method of reflections

In this section, I analyze the steady thermocapillary motion of a fluid sphere with relative thermal conductivity k^* and relative viscosity η^* either parallel to an infinite flat wall ($c \to \infty$) or on the median plane between two parallel plates ($c = b$), as shown in Fig. 4.1, by a method of reflections. The effect of the walls on the droplet velocity is sought in expansions of λ, which equals a/b, the ratio of the droplet radius to the distance between the walls and the center of the droplet.

C3.1. *Motion parallel to an infinite plane wall*

For the problem of thermocapillary motion parallel to an insulated plane wall, the governing equations in [4.1a] and [4.9] must be solved by satisfying the boundary conditions [4.2a-d] and [4.11b, c] with $c \to \infty$. The method-of-reflection solution consists of the following series, whose terms depend on increasing powers of λ:

$$T = T_0 + E_\infty x + T_{\mathrm{p}}^{(1)} + T_{\mathrm{w}}^{(1)} + T_{\mathrm{p}}^{(2)} + T_{\mathrm{w}}^{(2)} + \ldots, \qquad \text{[C3-1a]}$$

$$\mathrm{v} = \mathrm{v}_{\mathrm{p}}^{(1)} + \mathrm{v}_{\mathrm{w}}^{(1)} + \mathrm{v}_{\mathrm{p}}^{(2)} + \mathrm{v}_{\mathrm{w}}^{(2)} + \ldots, \qquad \text{[C3-1b]}$$

where subscripts w and p represent the reflections from wall and droplet, respectively, and the superscript (i) denotes the ith reflection from that surface. In these series, all the expansion sets of the corresponding temperature and velocity for the external fluid must satisfy [4.1a] and [4.9]. The advantage of this method is that it is necessary to consider boundary conditions associated with only one surface at a time.

According to [C3-1], the thermocapillary migration velocity of the droplet can also be expressed in the series form,

$$\mathrm{U} = U_0 \mathrm{e}_x + \mathrm{U}^{(1)} + \mathrm{U}^{(2)} + \ldots. \qquad \text{[C3-2]}$$

In this expression, U_0 is the thermocapillary velocity of an identical droplet suspended freely in the continuous phase far from the wall given by [1-4.1]; $\mathrm{U}^{(i)}$ is related to $\nabla T_{\mathrm{w}}^{(i)}$ and $\mathrm{v}_{\mathrm{w}}^{(i)}$ by (Anderson, 1985; Chen and Keh, 1990)

$$\mathrm{U}^{(i)} = A\frac{a}{\eta}\left(-\frac{\partial \gamma}{\partial T}\right)[\nabla T_{\mathrm{w}}^{(i)}]_0 + [\mathrm{v}_{\mathrm{w}}^{(i)}]_0 + C\frac{a^2}{6}[\nabla^2 \mathrm{v}_{\mathrm{w}}^{(i)}]_0\,. \qquad \text{[C3-3]}$$

Here, $A = 2(2+k^*)^{-1}(2+3\eta^*)^{-1}$, $C = 3\eta^*(2+3\eta^*)^{-1}$, and the subscript 0 to variables inside brackets denotes evaluation at the position of the droplet center. Note that $0 \le A \le 1/2$ and $0 \le C \le 1$. The last two terms in [C3-3] represent the Faxen law for the isothermal motion of a force-free fluid sphere (Hetsroni and Haber, 1970).

The solution for the first reflected fields from the droplet is

$$T_{\mathrm{p}}^{(1)} = GE_\infty a^3 r^{-2} \sin\theta \cos\phi, \quad \text{[C3-4a]}$$

$$\mathrm{v}_{\mathrm{p}}^{(1)} = \frac{1}{2} U_0 a^3 r^{-3} (2\sin\theta\cos\phi\, \mathrm{e}_r - \cos\theta\cos\phi\, \mathrm{e}_\theta + \sin\phi\, \mathrm{e}_\phi) , \quad \text{[C3-4b]}$$

Where $G = (1-k^*)(2+k^*)^{-1}$. Obviously, $-1 \le G \le 1/2$, with the upper and lower bounds occurring at the limits $k^* = 0$ and $k^* \to \infty$, respectively. The velocity distribution shown in [C3-4b] is identical to the irrotational flow surrounding a rigid sphere moving with velocity $U_0 \mathrm{e}_x$.

The boundary conditions for the *i*th reflected fields from the wall are derived from [4.2c, d] and [4.11d, e],

$$z = -b: \qquad \frac{\partial T_{\mathrm{w}}^{(i)}}{\partial z} = -\frac{\partial T_{\mathrm{p}}^{(i)}}{\partial z} , \quad \text{[C3-5a]}$$

$$\mathrm{v}_{\mathrm{w}}^{(i)} = -\mathrm{v}_{\mathrm{p}}^{(i)} ; \quad \text{[C3-5b]}$$

$$r \to \infty , \quad z > -b: \qquad T_{\mathrm{w}}^{(i)} \to 0 , \quad \text{[C3-5c]}$$

$$\mathrm{v}_{\mathrm{w}}^{(i)} \to 0 . \quad \text{[C3-5d]}$$

The solution of $T_{\mathrm{w}}^{(1)}$ is obtained by applying complex Fourier transforms on *x* and *y* in [4.1a] and [C3-5a, c], with the result

$$T_{\mathrm{w}}^{(1)} = GE_\infty a^3 x [x^2 + y^2 + (z+2b)^2]^{-3/2} . \quad \text{[C3-6a]}$$

This reflected temperature field may be interpreted as arising from the reflection of the imposed field $E_\infty \mathrm{e}_x$ from a fictitious droplet identical to the actual droplet, its location being at the mirror-image position of the actual droplet with respect to the plane $z = -b$ (i.e. at $x = 0, y = 0, z = -2b)$. The solution of $\mathrm{v}_{\mathrm{w}}^{(1)}$ can be found by fitting the boundary conditions [C3-5b, d] with the general solution to [4.9] established by Faxen (Happel and Brenner, 1983), which results in

$$\mathrm{v}_{\mathrm{w}}^{(1)} = \frac{U_0 a^3}{4\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i(\alpha x+\beta y)-\kappa(z+2b)}\{-[2\kappa(z+b)+1]i\alpha\,\mathrm{e}_z$$

$$-[2\kappa(z+b)-1](\frac{\alpha^2}{\kappa}\mathrm{e}_x + \frac{\alpha\beta}{\kappa}\mathrm{e}_y)\}d\alpha\, d\beta\,, \qquad \text{[C3-6b]}$$

where $\kappa = (\alpha^2+\beta^2)^{1/2}$, and $i = \sqrt{-1}$.

The contributions of $T_{\mathrm{w}}^{(1)}$ and $\mathrm{v}_{\mathrm{w}}^{(1)}$ to the droplet velocity are determined by using [C3-3],

$$\mathrm{U}_{\mathrm{t}}^{(1)} = A\frac{a}{\eta}(-\frac{\partial\gamma}{\partial T})[\nabla T_{\mathrm{w}}^{(1)}]_{r=0} = \frac{1}{8}G\lambda^3 U_0 \mathrm{e}_x\,, \qquad \text{[C3-7a]}$$

$$\mathrm{U}_{\mathrm{h}}^{(1)} = [\mathrm{v}_{\mathrm{w}}^{(1)} + C\frac{a^2}{6}\nabla^2 \mathrm{v}_{\mathrm{w}}^{(1)}]_{r=0} = -\frac{1}{8}(\lambda^3 - C\lambda^5)U_0\mathrm{e}_x\,, \qquad \text{[C3-7b]}$$

$$\mathrm{U}^{(1)} = \mathrm{U}_{\mathrm{t}}^{(1)} + \mathrm{U}_{\mathrm{h}}^{(1)} = \frac{1}{8}[-(1-G)\lambda^3 + C\lambda^5]U_0\mathrm{e}_x\,. \qquad \text{[C3-7c]}$$

Equation [C3-7a] shows that the reflected temperature field from the insulated wall can increase (if $G>0$ or $k^*<1$) or decrease (if $G<0$ or $k^*>1$) the velocity of the thermocapillary droplet, while [C3-7b] indicates that the reflected velocity field is to decrease this velocity; the net effect of the reflected fields is expressed by [C3-7c], which can enhance or retard the movement of the droplet, depending on the combination of the values of G (or k^*), η^*, and λ. When $G=0$ (or $k^*=1$), the reflected temperature field makes no contribution to the thermocapillary migration velocity. Equation [C3-7] indicates that the wall correction to the velocity of the thermocapillary droplet is $\mathrm{O}(\lambda^3)$, which is weaker than that obtained for the corresponding sedimentation problem, in which the leading boundary effect is $\mathrm{O}(\lambda)$. Note that the wall effect on thermocapillary motion involving the viscosity parameter η^* appears starting from $\mathrm{O}(\lambda^5)$, and the normalized droplet velocity increases with an increase in η^*. The necessary conditions for the wall enhancement on the thermocapillary motion to occur are a small value of k^*, a large value of η^*, and a value of λ close to unity such that the relation $C\lambda^5 > (1-G)\lambda^3$ is warranted.

The solution for the second reflected fields from the droplet is

$$T_{\mathrm{p}}^{(2)} = \frac{1}{8}E_\infty[G^2\lambda^3 a^3 r^{-2}\sin\theta\cos\phi + GH\lambda^4 a^4 r^{-3}\cos\theta\sin\theta\cos\phi + \mathrm{O}(\lambda^5 a^5)]\,,$$

[C3-8a]

$$\mathrm{v}_{\mathrm{p}}^{(2)} = \frac{1}{32}U_0[2G\lambda^3 a^3 r^{-3}(2\sin\theta\cos\phi\,\mathrm{e}_r - \cos\theta\cos\phi\,\mathrm{e}_\theta + \sin\phi\,\mathrm{e}_\phi)$$

$$-3(D-2G\frac{B}{A})\lambda^4 a^2 r^{-2}\cos\theta\sin\theta\cos\phi\,\mathrm{e}_r + \mathrm{O}(\lambda^4 a^4, \lambda^5 a^3)]\,. \qquad \text{[C3-8b]}$$

Here, $H = 3(1-k^*)(3+2k^*)^{-1}$, $B = 3(3+2k^*)^{-1}(1+\eta^*)^{-1}$, and $D = 3(2+5\eta^*)(1+\eta^*)^{-1}$.

The boundary conditions for the second reflected fields from the wall are obtained by substituting the results of $T_\mathrm{p}^{(2)}$ and $\mathrm{v}_\mathrm{p}^{(2)}$ into [C3-5], with which [4.1a] and [4.9] can be solved as before to yield

$$[\nabla T_\mathrm{w}^{(2)}]_{r=0} = [\frac{1}{64} G^2 \lambda^6 + \mathrm{O}(\lambda^8)] E_\infty \mathrm{e}_x \,, \qquad \text{[C3-9a]}$$

$$[\mathrm{v}_\mathrm{w}^{(2)}]_{r=0} = \{-\frac{1}{256}[3D - 2(3\frac{B}{A} - 2)G]\lambda^6 + \mathrm{O}(\lambda^8)\} U_0 \mathrm{e}_x \,. \qquad \text{[C3-9b]}$$

The contribution of the second reflected fields to the droplet velocity is obtained by putting $T_\mathrm{w}^{(2)}$ and $\mathrm{v}_\mathrm{w}^{(2)}$ into [C3-3], which gives

$$\mathrm{U}^{(2)} = \{-\frac{1}{256}[3D - 2(3\frac{B}{A} - 2)G - 4G^2]\lambda^6 + \mathrm{O}(\lambda^8)\} U_0 \mathrm{e}_x \,. \qquad \text{[C3-10]}$$

The errors for $\mathrm{U}^{(2)}$ is $\mathrm{O}(\lambda^8)$, because the $\mathrm{O}(\lambda^7)$ terms in the expansions of $\nabla T_\mathrm{w}^{(2)}$ and $\mathrm{v}_\mathrm{w}^{(2)}$ vanish at the center of the droplet.

Obviously, $\mathrm{U}^{(3)}$ will be $\mathrm{O}(\lambda^9)$. With the substitution of [C3-7c] and [C3-10] into [C3-2], the droplet velocity can be expressed as $\mathrm{U} = U \mathrm{e}_x$ with

$$U = U_0 \{1 - \frac{1}{8}(1-G)\lambda^3 + \frac{C}{8}\lambda^5$$

$$- \frac{1}{256}[3D - 2(3\frac{B}{A} - 2)G - 4G^2]\lambda^6 + \mathrm{O}(\lambda^8)\} \,. \qquad \text{[C3-11]}$$

The droplet migrates along the imposed temperature gradient at a rate that can increase or decrease as the droplet approaches the wall. Owing to the neglect of the inertial effect, the wall does not deflect the direction of thermocapillary migration.

For the case that a linear temperature profile is prescribed on the plane wall which is consistent with the far-field distribution ,namely, the boundary condition [4.2c] is replaced by [4.2e], the series expansions [C3-1] and [C3-2], the solution of $T_\mathrm{p}^{(1)}$ and $\mathrm{v}_\mathrm{p}^{(1)}$ in [C3-4], and the boundary conditions for $T_\mathrm{w}^{(i)}$ and $\mathrm{v}_\mathrm{w}^{(i)}$ in [C3-5b-d] are still valid, while [C3-5a] becomes

$$z = -b: \qquad T_\mathrm{w}^{(i)} = -T_\mathrm{p}^{(i)} \,. \qquad \text{[C3-12]}$$

With this change, it can be shown that the results of the reflected fields and of the droplet velocity are also obtained from [C3-6]-[C3-11] by replacing G by $-G$. Thus, contrary to the effect of an insulated plane wall, the reflected temperature field from a parallel wall with the imposed far-field temperature gradient reduces the droplet velocity if $G>0$ or $k^*<1$ and enhances this velocity if $G<0$ or $k^*>1$. When $G=0$ or $k^*=1$, the two types of plane wall will produce the same effects on the thermocapillary motion of the droplet. Under the conditions that the values of k^*, η^* and λ are sufficiently large such that $C\lambda^5>(1+G)\lambda^3$, the net effect of a lateral plane wall prescribed with the far-field temperature distribution can enhance the thermocapillary migration of a droplet.

C3.2. *Motion on the median plane between two parallel flat walls*

For the problem of thermocapillary motion on the median plane between two insulated parallel plates, the boundary conditions corresponding to governing equations [4.1a] and [4.9] are given by [4.2a-d] and [4.11b, c] with $c=b$. With $\lambda=a/b<<1$, the series expansions of the temperature, fluid velocity, and droplet velocity given by [C3-1]-[C3-4] remain valid here. From [4.2c, d] and [4.11d, e], the boundary conditions for $T_\mathrm{w}^{(i)}$ and $\mathrm{v}_\mathrm{w}^{(i)}$ are found to be

$$|z|=b: \qquad \frac{\partial T_\mathrm{w}^{(i)}}{\partial z}=-\frac{\partial T_\mathrm{p}^{(i)}}{\partial z}, \qquad \text{[C3-13a]}$$

$$\mathrm{v}_\mathrm{w}^{(i)}=-\mathrm{v}_\mathrm{p}^{(i)}; \qquad \text{[C3-13b]}$$

$$r\to\infty,\ |z|\le b: \qquad T_\mathrm{w}^{(i)}\to 0, \qquad \text{[C3-13c]}$$

$$\mathrm{v}_\mathrm{w}^{(i)}\to 0. \qquad \text{[C3-13d]}$$

The first wall-reflected fields can be solved by the same method as used for a single lateral plate in the previous subsection , with the results

$$T_\mathrm{w}^{(1)}=-\frac{GE_\infty a^3}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{i\alpha}{\kappa}e^{i(\alpha x+\beta y)-\kappa b}\frac{\cosh(\kappa z)}{\sinh(\kappa b)}d\alpha\, d\beta, \qquad \text{[C3-14a]}$$

$$\mathrm{v}_\mathrm{w}^{(1)}=\frac{U_0 a^3}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{\sinh(2\kappa b)-2\kappa b}e^{i(\alpha x+\beta y)}$$
$$\{[\sinh(\kappa z)-\kappa z\cosh(\kappa z)+g\sinh(\kappa z)]i\alpha \mathrm{e}_z$$
$$+[\kappa z\sinh(\kappa z)-g\cosh(\kappa z)](\frac{\alpha^2}{\kappa}\mathrm{e}_x+\frac{\alpha\beta}{\kappa}\mathrm{e}_y)\}d\alpha\, d\beta, \qquad \text{[C3-14b]}$$

where $\kappa=(\alpha^2+\beta^2)^{1/2}$ and $g=\kappa b-e^{-\kappa b}\sinh(\kappa b)$. The contributions of $T_\mathrm{w}^{(1)}$ and $\mathrm{v}_\mathrm{w}^{(1)}$ to the droplet velocity are determined using [C3-3], which lead to a result similar to [C3-7],

$$\mathrm{U}_\mathrm{t}^{(1)}=d_1 G\lambda^3 U_0\,\mathrm{e}_x, \qquad \text{[C3-15a]}$$

$$\mathrm{U}_\mathrm{h}^{(1)}=-(d_2\lambda^3-d_3 C\lambda^5)U_0\,\mathrm{e}_x, \qquad \text{[C3-15b]}$$

$$\mathrm{U}^{(1)}=\mathrm{U}_\mathrm{t}^{(1)}+\mathrm{U}_\mathrm{h}^{(1)}=[-(d_2-d_1 G)\lambda^3+d_3 C\lambda^5]U_0\mathrm{e}_x, \qquad \text{[C3-15c]}$$

where

$$d_1 = \int_0^\infty \frac{\rho^2}{e^{2\rho}-1} d\rho = 0.300514\,, \qquad \text{[C3-16a]}$$

$$d_2 = \frac{1}{2}\int_0^\infty \frac{\rho^2(\rho - e^{-\rho}\sinh\rho)}{\sinh(2\rho)-2\rho} d\rho = 0.417956\,, \qquad \text{[C3-16b]}$$

$$d_3 = \frac{1}{6}\int_0^\infty \frac{\rho^4}{\sinh(2\rho)-2\rho} d\rho = 0.338324\,. \qquad \text{[C3-16c]}$$

Analogous to the previous case, the results of the second reflections can be obtained as

$$T_{\mathrm{p}}^{(2)} = E_\infty[d_1 G^2 \lambda^3 a^3 r^{-2} \sin\theta\cos\phi + \mathrm{O}(\lambda^5 a^5)]\,, \qquad \text{[C3-17a]}$$

$$\mathrm{v}_{\mathrm{p}}^{(2)} = \frac{U_0}{2}[d_1 G \lambda^3 a^3 r^{-3}(2\sin\theta\cos\phi\, \mathrm{e}_r - \cos\theta\cos\phi\, \mathrm{e}_\theta + \sin\phi\, \mathrm{e}_\phi) + \mathrm{O}(\lambda^5 a^3)]\,,$$

[C3-17b]

$$[\nabla T_{\mathrm{w}}^{(2)}]_{r=0} = [d_1^2 G^2 \lambda^6 + \mathrm{O}(\lambda^8)] E_\infty \mathrm{e}_x\,, \qquad \text{[C3-18a]}$$

$$[\mathrm{v}_{\mathrm{w}}^{(2)}]_{r=0} = [-d_1 d_2 G \lambda^6 + \mathrm{O}(\lambda^8)] U_0 \mathrm{e}_x\,, \qquad \text{[C3-18b]}$$

and

$$\mathrm{U}^{(2)} = [-(d_1 d_2 G - d_1^2 G^2)\lambda^6 + \mathrm{O}(\lambda^8)] U_0 \mathrm{e}_x\,. \qquad \text{[C3-19]}$$

Note that the $\lambda^4 a^2$ and $\lambda^4 a^4$ terms in the expressions for $T_{\mathrm{p}}^{(2)}$ and $\mathrm{v}_{\mathrm{p}}^{(2)}$ vanish. With the combination of [C3-2], [C3-15], and [C3-19], the droplet velocity can be expressed as $\mathrm{U} = U\mathrm{e}_x$ with

$$U = U_0[1 - (d_2 - d_1 G)\lambda^3 + d_3 C \lambda^5 - (d_1 d_2 G - d_1^2 G^2)\lambda^6 + \mathrm{O}(\lambda^8)]. \qquad \text{[C3-20]}$$

For the case that the droplet is undergoing thermocapillary migration on the median plane between two parallel plates on which a linear temperature profile consistent with the far-field distribution is imposed, [4.2c] should be replaced by [4.2e]. In this case, [C3-1]-[C3-4] and [C3-13b-d] are still applicable, while [C3-13a] becomes

$$|z| = b: \qquad T_{\mathrm{w}}^{(i)} = -T_{\mathrm{p}}^{(i)}\,. \qquad \text{[C3-21]}$$

With this change, it can be shown that the results of the reflected fields and of the droplet velocity are also obtained from [C3-14]-[C3-20] by replacing G and d_1 by $-G$ and $\bar{d}_1$, respectively, where

$$\bar{d}_1 = \int_0^\infty \frac{\rho^2}{e^{2\rho}+1} d\rho = 0.225386\,. \qquad \text{[C3-22]}$$

Comparing [C3-19] for the slit case with [C3-11] for the case of a single parallel plane, one can find that the wall effects on the thermocapillary motion of a droplet in the two cases are qualitatively similar. However, the assumption that the result of the boundary effect for two walls can be obtained by simple addition of the single-wall effect generally gives a smaller correction to thermocapillary motion, while for the corresponding sedimentation problem this approximation overestimates the wall correction (Happel and Brenner, 1983).

C4. Analysis of the thermophoresis of a spherical particle parallel to plane walls by a method of reflections

In this section, I analyze the steady thermophoretic motion of an aerosol sphere with the relative thermal conductivity k^*, temperature jump coefficient C_t^*, and frictional slip coefficient C_m^* either parallel to an infinite flat wall ($c \to \infty$) or on the median plane between two parallel plates ($c = b$), as shown in Figure 5.1, by a method of reflections. The effect of the walls on the translational velocity U and angular velocity Ω of the particle is sought in expansions of λ, which equals a/b, the ratio of the particle radius to the distance between the wall and the center of the particle.

C4.1. *Motion parallel to an infinite plane wall*

For the problem of thermophoretic motion of a spherical particle parallel to an insulated plane wall, the governing Eqs. [5.1] and [5.9] must be solved by satisfying the boundary conditions [5.2a-d] and [5.10a-c] with $c \to \infty$. The method-of-reflection solution consists of the following series, whose terms depend on increasing powers of λ:

$$T = T_0 - E_\infty x + T_\mathrm{p}^{(1)} + T_\mathrm{w}^{(1)} + T_\mathrm{p}^{(2)} + T_\mathrm{w}^{(2)} + \ldots, \qquad \text{[C4-1a]}$$

$$\mathrm{v} = \mathrm{v}_\mathrm{p}^{(1)} + \mathrm{v}_\mathrm{w}^{(1)} + \mathrm{v}_\mathrm{p}^{(2)} + \mathrm{v}_\mathrm{w}^{(2)} + \ldots, \qquad \text{[C4-1b]}$$

where subscripts w and p represent the reflections from wall and particle, respectively, and the superscript (i) denotes the ith reflection from that surface. In these series, all the expansion sets of the corresponding temperature and velocity for the fluid phase must satisfy Eqs. [5.1a] and [5.9]. The advantage of this method is that it is necessary to consider boundary conditions associated with only one surface at a time.

According to Eq. [C4-1], the translational and angular velocities of the particle can also be expressed in the series form,

$$\mathrm{U} = U_0 \mathrm{e}_x + \mathrm{U}^{(1)} + \mathrm{U}^{(2)} + \ldots, \qquad \text{[C4-2a]}$$

$$\Omega = \Omega^{(1)} + \Omega^{(2)} + \dots \quad . \qquad \text{[C4-2b]}$$

In these expressions, $U_0 = AE_\infty$ is the thermophoretic velocity of an identical particle suspended freely in the continuous phase far from the wall given by Eqs. [1-5.1] and [1-5.2b]; $\mathrm{U}^{(i)}$ and $\Omega^{(i)}$ are related to $\nabla T_\mathrm{w}^{(i)}$ and $\mathrm{v}_\mathrm{w}^{(i)}$ by (Keh and Chen, 1995)

$$\mathrm{U}^{(i)} = A[\nabla T_\mathrm{w}^{(i)}]_0 + [\mathrm{v}_\mathrm{w}^{(i)}]_0 + \frac{a^2 D}{6}[\nabla^2 \mathrm{v}_\mathrm{w}^{(i)}]_0 \,, \qquad \text{[C4-3a]}$$

$$\Omega^{(i)} = \frac{1}{2}[\nabla \times \mathrm{v}_\mathrm{w}^{(i)}]_0 \,. \qquad \text{[C4-3b]}$$

Here, $D = (1 + 2C_\mathrm{m}^*)^{-1}$ and the subscript 0 to variables inside brackets denotes evaluation at the position of the particle center.

The solution for the first reflected fields from the particle is

$$T_\mathrm{p}^{(1)} = -GE_\infty a^3 r^{-2} \sin\theta \cos\phi, \qquad \text{[C4-4a]}$$

$$\mathrm{v}_\mathrm{p}^{(1)} = \frac{1}{2}U_0 a^3 r^{-3}(2\sin\theta\cos\phi\, \mathrm{e}_r - \cos\theta\cos\phi\, \mathrm{e}_\theta + \sin\phi\, \mathrm{e}_\phi) \,, \qquad \text{[C4-4b]}$$

where $G = (1 - k^* + k^* C_\mathrm{t}^*)(2 + k^* + 2k^* C_\mathrm{t}^*)^{-1}$. Obviously, $-1 \le G \le 1/2$, with the upper and lower bounds occuring at the limits $k^* = 0$ and $k^* \to \infty$ (when $C_\mathrm{t}^* << 1$), respectively. The velocity distribution shown in Eq. [C4-4b] is identical to the irrotational flow surrounding a rigid sphere moving with velocity $U_0 \mathrm{e}_x$.

The boundary conditions for the *i*th reflected fields from the wall are derived from Eqs. [5.2c], [5.2d], [5.10b], and [5.10c],

$$z = -b: \qquad \frac{\partial T_\mathrm{w}^{(i)}}{\partial z} = -\frac{\partial T_\mathrm{p}^{(i)}}{\partial z} \,, \qquad \text{[C4-5a]}$$

$$\mathrm{v}_\mathrm{w}^{(i)} = -\mathrm{v}_\mathrm{p}^{(i)} \,; \qquad \text{[C4-5b]}$$

$$r \to \infty \,, \quad z > -b: \qquad T_\mathrm{w}^{(i)} \to 0 \,, \qquad \text{[C4-5c]}$$

$$\mathrm{v}_\mathrm{w}^{(i)} \to 0 \,. \qquad \text{[C4-5d]}$$

The solution of $T_\mathrm{w}^{(1)}$ is obtained by applying complex Fourier transforms on *x* and *y* in Eqs. [5.4a] and [C4-5a, c] (taking $i = 1$), with the result

$$T_\mathrm{w}^{(1)} = -GE_\infty a^3 x[x^2 + y^2 + (z + 2b)^2]^{-3/2} \,. \qquad \text{[C4-6a]}$$

This reflected temperature field may be interpreted as arising from the reflection of the imposed field $-E_\infty \mathrm{e}_x$ from a fictitious particle identical to the actual particle, its location being at the mirror-image position of the actual particle with respect to the plane $z=-b$ (i.e. at $x=0, y=0, z=-2b$). The solution for $\mathrm{v}_\mathrm{w}^{(1)}$ can be found by fitting the boundary conditions Eqs. A5b, d with the general solution to Eq. [5.9] established by Faxen (Happel and Brenner, 1983, p. 323), which results in

$$\mathrm{v}_\mathrm{w}^{(1)} = \frac{U_0 a^3}{4\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\mathrm{i}(\alpha x+\beta y)-\kappa(z+2b)}\{-[2\kappa(z+b)+1]\mathrm{i}\,\alpha\,\mathrm{e}_z$$

$$-[2\kappa(z+b)-1](\frac{\alpha^2}{\kappa}\mathrm{e}_x + \frac{\alpha\beta}{\kappa}\mathrm{e}_y)\}\,\mathrm{d}\alpha\,\mathrm{d}\beta\,, \qquad \text{[C4-6b]}$$

where $\kappa = (\alpha^2+\beta^2)^{1/2}$ and $\mathrm{i}=\sqrt{-1}$.

The contributions of $T_\mathrm{w}^{(1)}$ and $\mathrm{v}_\mathrm{w}^{(1)}$ to the translational and angular velocities of the particle are determined by using Eq. [C4-3],

$$\mathrm{U}_\mathrm{t}^{(1)} = A[\nabla T_\mathrm{w}^{(1)}]_{r=0} = \frac{1}{8}G\lambda^3 U_0 \mathrm{e}_x\,, \qquad \text{[C4-7a]}$$

$$\mathrm{U}_\mathrm{h}^{(1)} = [\mathrm{v}_\mathrm{w}^{(1)} + \frac{a^2 D}{6}\nabla^2 \mathrm{v}_\mathrm{w}^{(1)}]_{r=0} = -\frac{1}{8}(\lambda^3 - D\lambda^5)U_0\mathrm{e}_x\,, \qquad \text{[C4-7b]}$$

$$\mathrm{U}^{(1)} = \mathrm{U}_\mathrm{t}^{(1)} + \mathrm{U}_\mathrm{h}^{(1)} = \frac{1}{8}[-(1-G)\lambda^3 + D\lambda^5]U_0\mathrm{e}_x\,, \qquad \text{[C4-7c]}$$

$$a\Omega^{(1)} = \frac{a}{2}[\nabla\times \mathrm{v}_\mathrm{w}^{(1)}]_{r=0} = -\frac{3}{16}U_0\lambda^4\mathrm{e}_y\,. \qquad \text{[C4-7d]}$$

Eq. [C4-7a] shows that the reflected temperature field from the insulated wall can increase (if $G>0$ or $k^* < (1-C_\mathrm{t}^*)^{-1}$) or decrease (if $G<0$ or $k^* > (1-C_\mathrm{t}^*)^{-1}$) the velocity of the thermophoretic particle, while Eq. [C4-7b] indicates that the reflected velocity field is to decrease this velocity; the net effect of the reflected fields is expressed by Eq. [C4-7c], which can enhance or retard the movement of the particle, depending on the combination of the values of G (or k^* and C_t^*), D (or C_m^*), and λ. When $G=0$ (or $k^* = (1-C_\mathrm{t}^*)^{-1}$), the reflected temperature field makes no contribution to the thermophoretic velocity. Eq. [C4-7c] indicates that the wall correction to the translational velocity of the thermophoretic particle is $\mathrm{O}(\lambda^3)$, which is weaker than that obtained for the corresponding sedimentation problem, in which the leading boundary effect is $\mathrm{O}(\lambda)$. Note that, when the values of

C_t^* and C_m^* are small, the necessary condition for the wall enhancement on the thermophoretic motion to occur is a small value of k^* and a value of λ close to unity such that the relation $D\lambda^5 > (1-G)\lambda^3$ is warranted.

Eq. [C4-7d] shows that the thermophoretic sphere rotates about an axis which is perpendicular to the direction of applied gradient and parallel to the plane wall. The direction of rotation is opposite to that which would occur if the sphere were driven to move by a body force. Note that the angular velocity $\Omega^{(1)}$ in Eq. [C4-7d] does not depend on the parameters G and D (since $\mathrm{v}_\mathrm{w}^{(1)}$ is not a function of G and D). Also, the wall-induced angular velocity of the thermophoretic particle is $\mathrm{O}(\lambda^4)$, which is the same in order as but different in its coefficient ($-3/16$ versus $3/32$) from that of a rigid sphere moving under a body-force field (Happel and Brenner, 1983, p. 327).

The solution for the second reflected fields from the particle is

$$T_\mathrm{p}^{(2)} = -\frac{1}{8}E_\infty[G^2\lambda^3a^3r^{-2}\sin\theta\cos\phi + 3GH\lambda^4a^4r^{-3}\cos\theta\sin\theta\cos\phi + \mathrm{O}(\lambda^5a^5)], \tag{C4-8a}$$

$$\begin{aligned}\mathrm{v}_\mathrm{p}^{(2)} = \frac{1}{32}U_0[&-2G\lambda^3a^3r^{-3}(2\sin\theta\cos\phi\,\mathrm{e}_r - \cos\theta\cos\phi\,\mathrm{e}_\theta + \sin\phi\,\mathrm{e}_\phi) \\ &+ (\frac{3}{2}G\frac{B}{A} + \frac{15}{8}C_1)\lambda^4a^2r^{-2}\cos\theta\sin\theta\cos\phi\,\mathrm{e}_r \\ &+ \frac{3}{32}C_2\lambda^4a^2r^{-2}(\cos\phi\,\mathrm{e}_\theta - \cos\theta\sin\phi\,\mathrm{e}_\phi) + \mathrm{O}(\lambda^4a^4, \lambda^5a^3)].\end{aligned} \tag{C4-8b}$$

Here, $H = \alpha_1(1-k^* + 2k^*C_t^*)$, $B = (5C_s\eta/2\rho_f T_0)\alpha_1\alpha_2(1+2k^*C_t^*)$, $C_1 = \alpha_2(1+2C_m^*)$, and $C_2 = (1+3C_m^*)^{-1}$, with $\alpha_1 = (3+2k^* + 6k^*C_t^*)$ and $\alpha_2 = (1+5C_m^*)^{-1}$.

The boundary conditions for the second reflected fields from the wall are obtained by substituting the results of $T_\mathrm{p}^{(2)}$ and $\mathrm{v}_\mathrm{p}^{(2)}$ into Eq. [C4-5], with which Eqs. [C4-4a] and [C4-15] can be solved as before to yield

$$[\nabla T_\mathrm{w}^{(2)}]_{r=0} = -[\frac{1}{64}G^2\lambda^6 + \mathrm{O}(\lambda^8)]E_\infty\mathrm{e}_x, \tag{C4-9a}$$

$$[\mathrm{v}_\mathrm{w}^{(2)}]_{r=0} = \{-\frac{1}{256}[4G(1+9\frac{B}{A}) - 45C_1]\lambda^6 + \mathrm{O}(\lambda^8)\}U_0\mathrm{e}_x. \tag{C4-9b}$$

The contribution of the second reflected fields to the translational and angular velocities of the particle is obtained by putting $T_{\mathrm{w}}^{(2)}$ and $\mathrm{v}_{\mathrm{w}}^{(2)}$ into Eq. [C4-3], which gives

$$\mathrm{U}^{(2)} = \{\frac{1}{256}[4G^2 - 4G(1+9\frac{B}{A}) - 45C_1]\lambda^6 + \mathrm{O}(\lambda^8)\}U_0\mathrm{e}_x\,, \qquad \text{[C4-10a]}$$

$$a\Omega^{(2)} = [-\frac{1}{1024}(18G + 72\frac{B}{A}G + 90C_1 + 15C_2)\lambda^7 + \mathrm{O}(\lambda^9)]U_0\,\mathrm{e}_y\,. \qquad \text{[C4-10b]}$$

The errors for $\mathrm{U}^{(2)}$ and $a\Omega^{(2)}$ are $\mathrm{O}(\lambda^8)$ and $\mathrm{O}(\lambda^9)$, respectively, because the $\mathrm{O}(\lambda^7)$ terms in the expansions of $\nabla T_{\mathrm{w}}^{(2)}$ and $\mathrm{v}_{\mathrm{w}}^{(2)}$ vanish at the position of the particle center.

Obviously, $\mathrm{U}^{(3)}$ and $a\Omega^{(3)}$ will be $\mathrm{O}(\lambda^9)$ and $\mathrm{O}(\lambda^{10})$, respectively. With the substitution of Eqs. [C4-7c,d] and [C4-10] into Eq. [C4-2], the particle velocities can be expressed as $\mathrm{U} = U\mathrm{e}_x$ and $\Omega = \Omega\mathrm{e}_y$ with

$$U = U_0\{1 - \frac{1}{8}(1-G)\lambda^3 + \frac{D}{8}\lambda^5$$

$$+\frac{1}{256}[4G^2 - 4(1+9\frac{B}{A})G - 45C_1]\lambda^6 + \mathrm{O}(\lambda^8)\}\,, \qquad \text{[C4-11a]}$$

$$a\Omega = U_0[-\frac{3}{16}\lambda^4 - \frac{1}{1024}(18G + 72\frac{B}{A}G + 90C_1 + 15C_2)\lambda^7 + O(\lambda^9)]\,. \qquad \text{[C4-11b]}$$

The particle migrates along the imposed temperature gradient at a rate that can increase or decrease as the particle approaches the wall. Owing to the neglect of inertial effects, the wall does not deflect the direction of thermophoresis.

For the case that a linear temperature profile is prescribed on the plane wall which is consistent with the far-field distribution, namely, the boundary condition Eq. [5.2c] is replaced by Eq. [5.2e], the series expansions [C4-1] and [C4-2], the solution of $T_{\mathrm{p}}^{(1)}$ and $\mathrm{v}_{\mathrm{p}}^{(1)}$ in Eq. [C4-4], and the boundary conditions for $T_{\mathrm{w}}^{(i)}$ and $\mathrm{v}_{\mathrm{w}}^{(i)}$ in Eqs. [C4-5b-d] are still valid, while Eq. [C4-5a] becomes

$$z = -b: \qquad T_{\mathrm{w}}^{(i)} = -T_{\mathrm{p}}^{(i)}\,. \qquad \text{[C4-12]}$$

With this change, it can be shown that the results of the reflected fields and of the particle velocities are also obtained from Eqs. [C4-6]-[C4-11] by replacing G by $-G$. Thus, contrary to the effect of an insulated plane wall, the reflected temperature field from a parallel wall with the imposed far-field temperature gradient reduces the translational velocity of the particle if $G>0$ or $k^*<(1-C_t^*)^{-1}$ and enhances this velocity if $G<0$ or $k^*>(1-C_t^*)^{-1}$. When $G=0$ or $k^*=(1-C_t^*)^{-1}$, the two types of plane wall will produce the same effects on the thermophoretic motion of the particle. Under the conditions that the values of C_t^* and C_m^* are small and the values of k^* and λ are sufficiently large such that $D\lambda^5>(1+G)\lambda^3$, the net effect of a lateral plane wall prescribed with the far-field temperature distribution can enhance the thermophoretic migration of a particle.

C4.2. *Motion on the median plane between two parallel flat walls*

For the problem of thermophoretic motion of a sphere on the median plane between two insulated parallel plates, the boundary conditions corresponding to governing Eqs. [5.1a] and [5.9] are given by Eqs. [5.2a-d] and [5.10a-c] with $c=b$. But, the angular velocity Ω of the particle vanishes now because of the symmetry. With $\lambda=a/b<<1$, the series expansions of the temperature, fluid velocity, and particle velocity given by Eqs. [C4-1], [C4-2a], and [C4-4] remain valid here. From Eqs. [5.2c], [5.2d], [5.10b], and [5.10c], the boundary conditions for $T_w^{(i)}$ and $\mathrm{v}_w^{(i)}$ are found to be

$$|z|=b: \qquad \frac{\partial T_w^{(i)}}{\partial z}=-\frac{\partial T_p^{(i)}}{\partial z}, \tag{C4-13a}$$

$$\mathrm{v}_w^{(i)}=-\mathrm{v}_p^{(i)}; \tag{C4-13b}$$

$$r\to\infty,\quad |z|\le b: \qquad T_w^{(i)}\to 0, \tag{C4-13c}$$

$$\mathrm{v}_w^{(i)}\to 0. \tag{C4-13d}$$

The first wall-reflected fields can be solved by the same method as used for a single lateral plate in the previous subsection , with the results

$$T_w^{(1)}=\frac{GE_\infty a^3}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{i}\alpha}{\kappa}e^{i(\alpha x+\beta y)-\kappa b}\frac{\cosh(\kappa z)}{\sinh(\kappa b)}\mathrm{d}\alpha\,\mathrm{d}\beta, \tag{C4-14a}$$

$$\mathrm{v}_w^{(1)}=\frac{U_0a^3}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{\sinh(2\kappa b)-2\kappa b}e^{\mathrm{i}(\alpha x+\beta y)}\{[-\kappa z\cosh(\kappa z)+(1+g)\sinh(\kappa z)]\mathrm{i}\alpha\mathrm{e}_z$$

$$+[\kappa z\sinh(\kappa z)-g\cosh(\kappa z)](\frac{\alpha^2}{\kappa}\mathrm{e}_x+\frac{\alpha\beta}{\kappa}\mathrm{e}_y)\}\mathrm{d}\alpha\,\mathrm{d}\beta, \tag{C4-14b}$$

where $\kappa=(\alpha^2+\beta^2)^{1/2}$ and $g=\kappa b-\mathrm{e}^{-\kappa b}\sinh(\kappa b)$. The contributions of $T_w^{(1)}$ and $\mathrm{v}_w^{(1)}$ to the particle velocity are determined using Eq. [C4-3a], which lead to a result similar to Eqs. [C4-7a-c],

$$\mathrm{U}_{\mathrm{t}}^{(1)} = d_1 G \lambda^3 U_0 \, \mathrm{e}_x \,, \qquad \text{[C4-15a]}$$

$$\mathrm{U}_{\mathrm{h}}^{(1)} = -(d_2 \lambda^3 - d_3 D \lambda^5) U_0 \, \mathrm{e}_x \,, \qquad \text{[C4-15b]}$$

$$\mathrm{U}^{(1)} = \mathrm{U}_{\mathrm{t}}^{(1)} + \mathrm{U}_{\mathrm{h}}^{(1)} = [-(d_2 - d_1 G)\lambda^3 + d_3 D \lambda^5] U_0 \mathrm{e}_x \,, \qquad \text{[C4-15c]}$$

where

$$d_1 = \int_0^\infty \frac{\rho^2}{\mathrm{e}^{2\rho} - 1} \mathrm{d}\,\rho = 0.300514 \,, \qquad \text{[C4-16a]}$$

$$d_2 = \frac{1}{2} \int_0^\infty \frac{\rho^2 (\rho - \mathrm{e}^{-\rho} \sinh \rho)}{\sinh(2\rho) - 2\rho} \mathrm{d}\,\rho = 0.417956 \,, \qquad \text{[C4-16b]}$$

$$d_3 = \frac{1}{6} \int_0^\infty \frac{\rho^4}{\sinh(2\rho) - 2\rho} \mathrm{d}\,\rho = 0.338324 \,. \qquad \text{[C4-16c]}$$

Analogous to the previous case, the results of the second reflections can be obtained as

$$T_{\mathrm{p}}^{(2)} = -E_\infty [d_1 G^2 \lambda^3 a^3 r^{-2} \sin\theta \cos\phi + \mathrm{O}(\lambda^5 a^5)] \,, \qquad \text{[C4-17a]}$$

$$\mathrm{v}_{\mathrm{p}}^{(2)} = \frac{U_0}{2} [d_1 G \lambda^3 a^3 r^{-3} (2 \sin\theta \cos\phi \, \mathrm{e}_r - \cos\theta \cos\phi \, \mathrm{e}_\theta + \sin\phi \, \mathrm{e}_\phi) + \mathrm{O}(\lambda^5 a^3)] \,,$$

[C4-17b]

$$[\nabla T_{\mathrm{w}}^{(2)}]_{r=0} = [d_1^2 G^2 \lambda^6 + \mathrm{O}(\lambda^8)] E_\infty \mathrm{e}_x \,, \qquad \text{[C4-18a]}$$

$$[\mathrm{v}_{\mathrm{w}}^{(2)}]_{r=0} = [-d_1 d_2 G \lambda^6 + \mathrm{O}(\lambda^8)] U_0 \mathrm{e}_x \,, \qquad \text{[C4-18b]}$$

and

$$\mathrm{U}^{(2)} = [-(d_1 d_2 G - d_1^2 G^2)\lambda^6 + \mathrm{O}(\lambda^8)] U_0 \mathrm{e}_x \,. \qquad \text{[C4-19]}$$

Note that the $\lambda^4 a^2$ and $\lambda^4 a^4$ terms in the expressions for $T_{\mathrm{p}}^{(2)}$ and $\mathrm{v}_{\mathrm{p}}^{(2)}$ vanish. With the combination of Eqs. [C4-2a], [C4-15c], and [C4-19], the particle velocity can be expressed as $\mathrm{U} = U \mathrm{e}_x$ with

$$U = U_0 [1 - (d_2 - d_1 G)\lambda^3 + d_3 D \lambda^5 - (d_1 d_2 G - d_1^2 G^2)\lambda^6 + \mathrm{O}(\lambda^8)] \,. \qquad \text{[C4-20]}$$

For the case that the particle is undergoing thermophoresis on the median plane between two parallel plates on which a linear temperature profile consistent with the far-field distribution is imposed, Eq. [5.2c] should be replaced by Eq. [5.2e]. In this case, Eqs. [C4-1], [C4-2a], [C4-4] and [C4-13b-d] are still applicable, while Eq. [C4-13a] becomes

$$|z| = b: \qquad T_{\mathrm{w}}^{(i)} = -T_{\mathrm{p}}^{(i)} \,. \qquad \text{[C4-21]}$$

With this change, it can be shown that the results of the reflected fields and of the particle velocity are also obtained from Eq. [C4-14]-[C4-20] by replacing G and d_1 by $-G$ and $\bar{d}_1$, respectively, where

$$\bar{d}_1 = \int_0^{\infty} \frac{\rho^2}{e^{2\rho}+1} \mathrm{d}\rho = 0.225386 . \qquad \text{[C4-22)]}$$

Comparing Eq. [C4-20] for the slit case with Eq. [C4-11a] for the case of a single parallel plane, one can find that the wall effects on the thermophoretic velocity of a particle in the two cases are qualitatively similar. However, the assumption that the result of the boundary effect for two walls can be obtained by simple addition of the single-wall effects generally gives a smaller correction to thermophoretic velocity, while for the corresponding sedimentation problem this approximation overestimates the wall correction.

References

Anderson, J. L., 1985. Droplet interactions in thermocapillary motion. *Int. J. Multiphase Flow*, **11**, 813.

Chen, S. H., Keh, H. J., 1990. Thermocapillary motion of a fluid droplet normal to a plane surface. *J. Colloid Interface Sci*., **137**, 550.

Happel, J., Brenner, H., 1983. *Low Reynolds Number Hydrodynamics.* Nijhoff. The Hague, The Netherlands.

Hetsroni, G., Haber, S., 1970. The flow in and around a droplet or bubble submerged in an unbound arbitrary velocity field. *Rheol. Acta.*, **9**, 488.

Keh, H. J., Chen, S. H., 1995. Particle Interactions in Thermophoresis. *Chem. Engng. Sci*., **50**, 3395.

Keh, H. J., Luo, S. C., 1995. Particle interactions in diffusiophoresis in nonelectrolyte gradients. *Physics of Fluids*, **7**, 2122.

Keh, H. J., Tu, H. J., 2000. Osmophoresis in a dilute suspension of spherical vesicles. *Int. J. Multiphase Flow*, **26**, 125.

Appendix D Some complicated definitions of function

The functions $\delta_n^{(i)}$ with $i=1,\ 2,\ 3,$ and 4 in Eqs. [2.11], [2.12], [2.26], [3.10], [3.11], [3.18], [4.7], [4.8], [4.16e], [4.16f], [5.7], [5.8], and [5.13] are defined by

$$\delta_n^{(1)}(r,\mu)=r^{-n-1}P_n^1(\mu)-(-n)^m\int_0^\infty \kappa^{1-m}\frac{J_1(\kappa\rho)}{\sinh\tau}[c^2V_{n+m}(c)(\sinh\sigma)^{1-m}(\cosh\sigma)^m$$

$$-b^2V_{n+m}(-b)(\sinh\omega)^{1-m}(\cosh\omega)^m]\,\mathrm{d}\kappa\,, \qquad \text{[D1]}$$

$$\delta_n^{(2)}(r,\mu)=-(n+1)r^{-n-2}P_n^1(\mu)-(-n)^m\int_0^\infty \frac{\kappa^{2-m}}{\sinh\tau}\{J_1'(\kappa\rho)(1-\mu^2)^{1/2}$$

$$[c^2V_{n+m}(c)(\sinh\sigma)^{1-m}(\cosh\sigma)^m-b^2V_{n+m}(-b)(\sinh\omega)^{1-m}(\cosh\omega)^m]$$

$$+J_1(\kappa\rho)\mu[c^2V_{n+m}(c)(\cosh\sigma)^{1-m}(\sinh\sigma)^m$$

$$-b^2V_{n+m}(-b)(\cosh\omega)^{1-m}(\sinh\omega)^m]\}\,\mathrm{d}\kappa\,, \qquad \text{[D2]}$$

$$\delta_n^{(3)}(r,\mu)=-r^{-n-1}\frac{\partial P_n^1(\mu)}{\partial\mu}(1-\mu^2)^{1/2}-(-n)^m r\int_0^\infty \frac{\kappa^{2-m}}{\sinh\tau}\{J_1'(\kappa\rho)\mu$$

$$[c^2V_{n+m}(c)(\sinh\sigma)^{1-m}(\cosh\sigma)^m-b^2V_{n+m}(-b)(\sinh\omega)^{1-m}(\cosh\omega)^m]$$

$$-J_1(\kappa\rho)(1-\mu^2)^{1/2}[c^2V_{n+m}(c)(\cosh\sigma)^{1-m}(\sinh\sigma)^m$$

$$-b^2V_{n+m}(-b)(\cosh\omega)^{1-m}(\sinh\omega)^m]\}\,\mathrm{d}\kappa\,, \qquad \text{[D3]}$$

$$\delta_n^{(4)}(r,\mu)=(n+1)(n+2)r^{-n-3}P_n^1(\mu)$$

$$-(-n)^m\int_0^\infty \frac{\kappa^{3-m}}{\sinh\tau}\{[J_1''(\kappa\rho)(1-\mu^2)+J_1(\kappa\rho)\mu^2]$$

$$[-c^2V_{n+m}(\sinh\sigma)^{1-m}(\cosh\sigma)^m-b^2V_{n+m}(-b)(\sinh\omega)^{1-m}(\cosh\omega)^m]$$

$$+2J_1'(\kappa\rho)(1-\mu^2)^{1/2}\mu[c^2V_{n+m}(c)(\cosh\sigma)^{1-m}(\sinh\sigma)^m$$

$$-b^2V_{n+m}(-b)(\cosh\omega)^{1-m}(\sinh\omega)^m]\}\,\mathrm{d}\kappa\,. \qquad \text{[D4]}$$

Here,

$$V_n(z_i)=\frac{(2/\pi)^{1/2}}{z_i^{n+1}}\sum_{q=0}^{[n/2]}\frac{(\kappa|z_i|)^{n-q-\frac{1}{2}}}{(-2)^q q!(n-2q-1)!}K_{n-q-\frac{3}{2}}(\kappa|z_i|)\,, \qquad \text{[D5]}$$

$$\sigma=\kappa(z+b)\,,\qquad \omega=\kappa(z-c)\,,\qquad \tau=\kappa(b+c)\,,\qquad \rho=(x^2+y^2)^{1/2} \qquad \text{[D6a,b,c,d]}$$

J_ν is the Bessel function of the first kind of order ν and the prime on it denotes differentiation with respect to its argument, K_ν is the modified Bessel function of the second kind of order ν, and the square bracket $[\nu]$ denotes the largest integer which is less than or equal to ν. In Eqs. [D1]-[D4], $m=1$ if Eqs. [2.5], [3.3], [4.2c], and [5.2c] are used for the boundary condition of the solute concentration or temperature field at the plane walls and $m=0$ if Eqs. [2.7], [3.5], [4.2e], and [5.2e] are used.

The starred A_n, B_n, and C_n functions in Eqs. [4.16] and [5.13] are defined by

$$A_n^*(r,\mu,\phi)=(1-\mu^2)^{1/2}(A_n'+\alpha_n')\cos\phi+(1-\mu^2)^{1/2}(A_n''+\alpha_n'')\sin\phi+\mu(A_n'''+\alpha_n'''),\tag{D7a}$$

$$B_n^*(r,\mu,\phi)=(1-\mu^2)^{1/2}(B_n'+\beta_n')\cos\phi+(1-\mu^2)^{1/2}(B_n''+\beta_n'')\sin\phi+\mu(B_n'''+\beta_n'''),\tag{D7b}$$

$$C_n^*(r,\mu,\phi)=(1-\mu^2)^{1/2}(C_n'+\gamma_n')\cos\phi+(1-\mu^2)^{1/2}(C_n''+\gamma_n'')\sin\phi+\mu(C_n'''+\gamma_n'''),\tag{D7c}$$

$$A_n^{**}(r,\mu,\phi)=\mu(A_n'+\alpha_n')\cos\phi+\mu(A_n''+\alpha_n'')\sin\phi-(1-\mu^2)^{1/2}(A_n'''+\alpha_n'''),\tag{D7d}$$

$$B_n^{**}(r,\mu,\phi)=\mu(B_n'+\beta_n')\cos\phi+\mu(B_n''+\beta_n'')\sin\phi-(1-\mu^2)^{1/2}(B_n'''+\beta_n'''),\tag{D7e}$$

$$C_n^{**}(r,\mu,\phi)=\mu(C_n'+\gamma_n')\cos\phi+\mu(C_n''+\gamma_n'')\sin\phi-(1-\mu^2)^{1/2}(C_n'''+\gamma_n'''),\tag{D7f}$$

$$A_n^{***}(r,\mu,\phi)=-(A_n'+\alpha_n')\sin\phi+(A_n''+\alpha_n'')\cos\phi,\tag{D7g}$$

$$B_n^{***}(r,\mu,\phi)=-(B_n'+\beta_n')\sin\phi+(B_n''+\beta_n'')\cos\phi,\tag{D7h}$$

$$C_n^{***}(r,\mu,\phi)=-(C_n'+\gamma_n')\sin\phi+(C_n''+\gamma_n'')\cos\phi.\tag{D7i}$$

Here, the primed A_n, B_n, C_n, α_n, β_n, and γ_n are functions of position in Eqs. [4.13] and [5.12] defined by

$$A_n'=\frac{1}{2r^n}[2n(2n-1)\sin\theta P_n^1(\mu)\cos^2\phi+(n-2)P_{n-1}^2(\mu)\cos2\phi$$
$$-n(n+1)(n-2)P_{n-1}(\mu)],\tag{D8a}$$

$$B_n'=-\frac{1}{2r^{n+2}}[P_{n+1}^2(\mu)\cos2\phi-n(n+1)P_{n+1}(\mu)],\tag{D8b}$$

$$C_n'=\frac{1}{2r^{n+1}}[P_n^2(\mu)\cos2\phi+n(n+1)P_n(\mu)],\tag{D8c}$$

$$A_n''=\frac{1}{r^n}[n(2n-1)\sin\theta P_n^1(\mu)+(n-2)P_{n-1}^2(\mu)]\cos\phi\sin\phi,\tag{D8d}$$

$$B_n''=-\frac{1}{r^{n+2}}P_{n+1}^2(\mu)\cos\phi\sin\phi,\tag{D8e}$$

$$C_n'' = \frac{1}{r^{n+1}} P_n^2(\mu)\cos\phi\sin\phi\,, \tag{D8f}$$

$$A_n''' = \frac{1}{r^n}[n(2n-1)\mu P_n^1(\mu) - (n+1)(n-2)P_{n-1}^1(\mu)]\cos\phi\,, \tag{D8g}$$

$$B_n''' = -\frac{1}{r^{n+2}} nP_{n+1}^1(\mu)\cos\phi\,, \tag{D8h}$$

$$C_n''' = -\frac{1}{r^{n+1}} P_n^1(\mu)\cos\phi\,, \tag{D8i}$$

$$\alpha_n' = \int_0^\infty \{G_5(\omega)H_1(-b) - G_5(\sigma)H_1(c) + G_6(\sigma,\omega)H_2(-b) - G_6(\omega,\sigma)H_2(c)$$
$$+G_1(\sigma,\omega)H_3(-b) - G_1(\omega,\sigma)H_3(c)\}d\kappa\,, \tag{D9a}$$

$$\beta_n' = \int_0^\infty \{G_5(\omega)H_4(-b) - G_5(\sigma)H_4(c) + G_6(\sigma,\omega)H_5(-b) - G_6(\omega,\sigma)H_5(c)$$
$$+G_1(\sigma,\omega)H_6(-b) - G_1(\omega,\sigma)H_6(c)\}d\kappa\,, \tag{D9b}$$

$$\gamma_n' = \int_0^\infty \{G_5(\omega)H_7(-b) - G_5(\sigma)H_7(c) + G_6(\sigma,\omega)H_8(-b) - G_6(\omega,\sigma)H_8(c)$$
$$+G_1(\sigma,\omega)H_9(-b) - G_1(\omega,\sigma)H_9(c)\}d\kappa\,, \tag{D9c}$$

$$\alpha_n'' = \int_0^\infty \{G_6(\sigma,\omega)H_{10}(-b) - G_6(\omega,\sigma)H_{10}(c) + G_3(\sigma,\omega)H_{11}(-b) - G_3(\omega,\sigma)H_{11}(c)$$
$$+G_1(\sigma,\omega)H_{12}(-b) - G_1(\omega,\sigma)H_{12}(c)\}d\kappa\,, \tag{D9d}$$

$$\beta_n'' = \int_0^\infty \{G_6(\sigma,\omega)H_{13}(-b) - G_6(\eta,\omega)H_{13}(c) + G_3(\sigma,\omega)H_{14}(-b) - G_3(\omega,\sigma)H_{14}(c)$$
$$+G_1(\sigma,\omega)H_{15}(-b) - G_1(\omega,\sigma)H_{15}(c)\}d\kappa\,, \tag{D9e}$$

$$\gamma_n'' = \int_0^\infty \{G_6(\sigma,\omega)H_{16}(-b) - G_6(\omega,\sigma)H_{16}(c) + G_3(\sigma,\omega)H_{17}(-b) - G_3(\omega,\sigma)H_{17}(c)$$
$$+G_1(\sigma,\omega)H_{18}(-b) - G_1(\omega,\sigma)H_{18}(c)\}d\kappa\,, \tag{D9f}$$

$$\alpha_n''' = \int_0^\infty \{G_2(\sigma,\omega)H_{19}(-b) - G_2(\omega,\sigma)H_{19}(c) + G_4(\sigma,\omega)H_{20}(-b)$$
$$-G_4(\omega,\sigma)H_{20}(c)\}d\kappa\,, \tag{D9g}$$

$$\beta_n''' = \int_0^\infty \{G_2(\sigma,\omega)H_{21}(-b) - G_2(\omega,\sigma)H_{21}(c) + G_4(\sigma,\omega)H_{22}(-b)$$
$$-G_4(\omega,\sigma)H_{22}(c)\}d\kappa\,, \tag{D9h}$$

$$\gamma_n''' = \int_0^\infty \{G_2(\sigma,\omega)H_{23}(-b) - G_2(\omega,\sigma)H_{23}(c) + G_4(\sigma,\omega)H_{24}(-b)$$
$$-G_4(\omega,\sigma)H_{24}(c)\}d\kappa\,, \tag{D9i}$$

where

$$G_{1,2}(u,v) = 4\tau uv[\frac{\sinh u}{u} \pm \frac{\sinh\tau}{\tau}\frac{\sinh v}{v}]/\delta_2\,, \tag{D10a}$$

$$G_{3,4}(u,v)=4\tau\{v[\cosh u-\frac{\sinh\tau}{\tau}\frac{\sinh v}{v}]\pm u[\frac{\sinh u}{u}-\frac{\sinh\tau}{\tau}\cosh v]\}/\delta_2\,, \qquad \text{[D10b]}$$

$$G_5(u,v)=-2\sinh u/\delta_1\,, \qquad \text{[D10c]}$$

$$G_6(u,v)=8\tau^2\{u\frac{\sinh\tau}{\tau}[\frac{\sinh u}{u}-\frac{\sinh\tau}{\tau}\cosh v]$$

$$+v[\frac{\sinh\tau}{\tau}\cosh u-\frac{\sinh v}{v}]/\delta_1\delta_2\,. \qquad \text{[D10d]}$$

$$H_1(z_i)=-n(2n-1)z_i^2 J_0(\kappa\rho)B_{n,1,1,0}(z_i)+n(2n-1)\frac{z_i^2}{\rho^2}B_1B_{n,1,2,1}(z_i)$$

$$-\frac{1}{2}(n-2)(y^2-x^2)B_2B_{n-1,2,2,3}(z_i)+\frac{1}{2}n(n+1)(n-2)J_0(\kappa\rho)B_{n-1,0,0,1}(z_i)\,,$$

$$\text{[D11a]}$$

$$H_2(z_i)=\{-n(2n-1)z_i^2[B_{n,1,1,0}(z_i)-B_{n,1,2,1}(z_i)]+\frac{1}{2}(n-2)z_i^2B_{n-1,2,2,1}(z_i)$$

$$+\frac{1}{2}n(n+1)(n-2)B_{n-1,0,0,1}(z_i)\}\frac{B_1}{\rho^2}\,, \qquad \text{[D11b]}$$

$$H_3(z_i)=\kappa z_i^2[-n(2n-1)z_iB_{n,1,1,0}(z_i)+(n+1)(n-2)B_{n-1,1,1,0}(z_i)]\frac{B_1}{\rho^2}\,, \qquad \text{[D11c]}$$

$$H_4(z_i)=\frac{1}{2}[(y^2-x^2)B_2B_{n+1,2,2,3}(z_i)-n(n+1)J_0(\kappa\rho)B_{n+1,0,0,1}(z_i)]\,, \qquad \text{[D11d]}$$

$$H_5(z_i)=-\frac{1}{2}[z_i^2B_{n+1,2,2,1}(z_i)+n(n+1)B_{n+1,0,0,1}(z_i)]\frac{B_1}{\rho^2}\,, \qquad \text{[D11e]}$$

$$H_6(z_i)=n\frac{\kappa z_i^2}{\rho^2}B_1B_{n+1,1,1,0}(z_i)\,, \qquad \text{[D11f]}$$

$$H_7(z_i)=-\frac{1}{2}[(y^2-x^2)B_2B_{n+1,2,2,3}(z_i)+n(n+1)J_0(\kappa\rho)B_{n,0,0,1}(z_i)]\,, \qquad \text{[D11g]}$$

$$H_8(z_i)=\frac{1}{2}[z_i^2B_{n,2,2,1}(z_i)-n(n+1)B_{n,0,0,1}(z_i)]\frac{B_1}{\rho^2}\,, \qquad \text{[D11h]}$$

$$H_9(z_i)=\kappa z_i^2B_{n,1,1,0}(z_i)\frac{B_1}{\rho^2}\,, \qquad \text{[D11i]}$$

$$H_{10}(z_i)=xyB_2[-n(2n-1)B_{n,1,1,2}(z_i)-\frac{1}{2}(n-2)B_{n-1,2,2,3}(z_i)$$

$$+\frac{1}{2z_i^2}n(n+1)(n-2)B_{n-1,0,0,3}(z_i)]\,, \qquad \text{[D11j]}$$

$$H_{11}(z_i)=xyB_2[n(2n-1)B_{n,1,2,3}(z_i)+(n-2)B_{n-1,2,2,3}(z_i)]\,, \qquad \text{[D11k]}$$

$$H_{12}(z_i)=\kappa xyB_2[-n(2n-1)z_iB_{n,1,1,2}(z_i)+(n+1)(n-2)B_{n-1,1,1,2}(z_i)]\,, \qquad \text{[D11l]}$$

$$H_{13}(z_i)=\frac{1}{2}xyB_2[B_{n+1,2,2,3}(z_i)-n(n+1)\frac{1}{z_i^2}B_{n+1,0,0,3}(z_i)]\,, \qquad \text{[D11m]}$$

$$H_{14}(z_i)=-xyB_2B_{n+1,2,2,3}(z_i)\,, \qquad \text{[D11n]}$$

$$H_{15}(z_i) = n\kappa xyB_2B_{n+1,1,1,2}(z_i)\,, \qquad \text{[D11o]}$$

$$H_{16}(z_i) = -\frac{1}{2}xyB_2[B_{n,2,2,3}(z_i) + n(n+1)\frac{1}{z_i^2}B_{n,0,0,3}(z_i)], \qquad \text{[D11p]}$$

$$H_{17}(z_i) = xyB_2B_{n,2,2,3}(z_i)\,, \qquad \text{[D11q]}$$

$$H_{18}(z_i) = \kappa xyB_2B_{n,1,1,2}(z_i), \qquad \text{[D11r]}$$

$$H_{19}(z_i) = -x\frac{J_1(\kappa\rho)}{\kappa^2\rho}\{n(2n-1)[B_{n,1,1,2}(z_i) - B_{n,1,2,3}(z_i)]$$

$$-\frac{1}{2}(n-2)B_{n-1,2,2,3}(z_i) - \frac{1}{2}n(n+1)(n-2)\frac{1}{z_i^2}B_{n-1,0,0,3}(z_i)\}\,, \qquad \text{[D11s]}$$

$$H_{20}(z_i) = -x\frac{J_1(\kappa\rho)}{\kappa\rho}[n(2n-1)z_iB_{n,1,1,2}(z_i) - (n+1)(n-2)B_{n-1,1,1,2}(z_i)], \qquad \text{[D11t]}$$

$$H_{21}(z_i) = -\frac{1}{2}x\frac{J_1(\kappa\rho)}{\kappa^2\rho}[B_{n+1,2,2,3}(z_i) + n(n+1)\frac{1}{z_i^2}B_{n+1,0,0,3}(z_i)]\,, \qquad \text{[D11u]}$$

$$H_{22}(z_i) = nx\frac{J_1(\kappa\rho)}{\kappa\rho}B_{n+1,1,1,2}(z_i)\,, \qquad \text{[D11v]}$$

$$H_{23}(z_i) = \frac{1}{2}x\frac{J_1(\kappa\rho)}{\kappa^2\rho}[B_{n,2,2,3}(z_i) - n(n+1)\frac{1}{z_i^2}B_{n,0,0,3}(z_i)]\,, \qquad \text{[D11w]}$$

$$H_{24}(z_i) = x\frac{J_1(\kappa\rho)}{\kappa\rho}B_{n,1,1,2}(z_i)\,, \qquad \text{[D11x]}$$

and P_n^m is the associated Legendre function of order n and degree m and $\mu = \cos\theta$. In Eq. [D10], the subscripts 1, 3 and 2, 4 to *G* refer to the plus and minus signs, respectively, on the right-hand sides, *u* and *v* are dummy variables, $\delta_1 = 2\sinh\tau$, and $\delta_2 = 4[\sinh^2\tau - \tau^2]$. In Eq. [D11],

$$B_1 = x^2J_0(\kappa\rho) + (y^2 - x^2)\frac{J_1(\kappa\rho)}{\kappa\rho}\,, \qquad \text{[D12a]}$$

$$B_2 = \frac{1}{\kappa^2\rho^2}[J_0(\kappa\rho) - 2\frac{J_1(\kappa\rho)}{\kappa\rho}]\,, \qquad \text{[D12b]}$$

$$\rho = (x^2 + y^2)^{1/2}, \qquad \text{[D12c]}$$

$$B_{n,m,j,l}(z_i) = \sum_{q=0}^{[n/2]} S_{nmq}(z_i)(\kappa|z_i|)^{n-q+l-1/2}K_{n-q-j-1/2}(\kappa|z_i|)\,, \qquad \text{[D12d]}$$

and

$$S_{nmq}(z_i) = \frac{(2/\pi)^{1/2}}{(-2)^q q!(n-2q-m)!z_i^{n+m}}\,. \qquad \text{[D12e]}$$

Appendix E: Associated computer programming source code

Appendix E1-1: Computer programming source code for estimating the diffusio-phoretic velocity of single spherical particle parallel one solute impenetrable plate.

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION BF(900,3),WET(96)
      DIMENSION RAD(2),A(500,501),DDK(96),B(500,501)
      INTEGER GGG,T,GG,NX,LL1,LL2,LBB,LCC
      OPEN (23,FILE='GAUSS80.DAT',STATUS='OLD')
      OPEN (25,FILE='D-1.TXT',STATUS='NEW')
      OPEN (24,FILE='WET3.DAT',STATUS='OLD')
      IN=80
      BB=0.1D0
      DO 1001 I=1,IN
      READ (23,*) DDK(I),WET(I)
1001  CONTINUE
      T=1
      PI=DACOS(-1.D0)
      FI=.01*PI/180.
      U4=DCOS(FI)
      U5=DSIN(FI)
      DO 3231 IUY=1,50
      READ(24,*) CV,NX
      RAD(1)=CV*BB
      BETA=1.D0*RAD(1)
      GGG=T*NX
      DO 511 I=1,T
      DO 512 J=1,NX
      NU=J+NX*(I-1)
      DO 513 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      WRITE(*,*) R2,BETA
      B(NU,GGG+1)=-1*(1-BETA*2/R2)*(U3*U4)
      DO 514 N=1,NX
      NZ=N+NX*(K-1)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1)
      CALL XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3,SM4)
      B(NU,NZ)=(1-BETA*2/R2)*((-N-1)*R2**(-1*(N+2))*W1*U4+SM1)
     &-BETA*((N+1)*(N+2)*R2**(-1*(N+3))*W1*U4+SM2)
514   CONTINUE
513   CONTINUE
512   CONTINUE
511   CONTINUE

      LL1=500
      LL2=501
      LBB=GGG
      LCC=GGG+1
      CALL GAUSL(LL1,LL2,LBB,LCC,B)
      GG=T*NX
      DO 7765 NN=1,3
```

```
      DO 111 I=1,T
      DO 112 J=1,NX
      NO=J+NX*(I-1)
      NP=J+NX*(I-1)+T*NX
      NQ=J+NX*(I-1)+2*T*NX
      DO 113 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)

      IF(NN.EQ.1) THEN
      A(NO,3*GG+1)=1.D0
      A(NP,3*GG+1)=0.D0
      A(NQ,3*GG+1)=0.D0
      END IF

      IF(NN .EQ. 2) THEN
      A(NO,3*GG+1)=U2
      A(NP,3*GG+1)=0.D0
      A(NQ,3*GG+1)=-1*U3*U4
      END IF

      DO 114 N=1,NX
      NE=(3*N-2)+3*NX*(K-1)
      NF=(3*N-1)+3*NX*(K-1)
      NG=(3*N-0)+3*NX*(K-1)
      CALL FUCK1(U2,N,W,WW,WWW)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1)
      CALL FUCK3(U2,N,W2,WW2,WWW2)
      CALL XXD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SUM1,SUM2,SUM3,SUM4,
     & SUM5,SUM6,SUM7,SUM8,SUM9)
      A(NO,NE)=((2.*N*(2*N-1)*U3*W1*U4**2.+(N-2)*WW2*DCOS(2.*FI)-N*(N+1)
    &*(N-2)*WW)/2./R2**(N))+SUM1
      A(NO,NF)=(-1.*(WWW2*DCOS(2.*FI)-N*(N+1)*WWW)/2./R2**(N+2)+SUM2)
      A(NO,NG)=((W2*DCOS(2.*FI)+N*(N+1)*W)/2./R2**(N+1)+SUM3)
      A(NP,NE)=(N*(2*N-1)*U3*W1+(N-2)*WW2)*U4*U5/R2**(N)+SUM4
      A(NP,NF)=-(WWW2*U4*U5)/R2**(N+2)+SUM5
      A(NP,NG)=(W2*U4*U5)/R2**(N+1)+SUM6
      A(NQ,NE)=((N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U4/R2**N+SUM7)
      A(NQ,NF)=(-(N*WWW1*U4)/R2**(N+2)+SUM8)
      A(NQ,NG)=(-(W1*U4)/R2**(N+1)+SUM9)
114   CONTINUE
113   CONTINUE
112   CONTINUE
111   CONTINUE

      IF(NN.EQ.3)THEN
      DO 811 J=1,NX
      NO=J
      NP=J+NX
      NQ=J+2*NX
      CALL FU(1,J,1,NX,RAD,PI,U2,U3,R2)
      VALUE1=0.D0
      VALUE2=0.D0

      DO 713 KK=1,NX
      NZ=KK
      CALL FUCK2(U2,KK,W1,WW1,WWW1,PW1)
      CALL XRD(KK,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3,SM4)
      ZZ=RAD(1)*U2
```

```
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      VALUE1=VALUE1
     &+B(NZ,GGG+1)*(-1*RAD(1)**(-KK-2)*PW1*U3*U4+SM3/RAD(1))
      VALUE2=VALUE2
     &+B(NZ,GGG+1)*(-1*RAD(1)**(-KK-2)*W1*U5/U3+SM4/(RAD(1)*U3))

713   CONTINUE
      A(NO,3*GG+1)=-1*((U2*U4+VALUE1)*U2*U4+(-1*U5+VALUE2)*(-1*U5))
      A(NP,3*GG+1)=-1*((U2*U4+VALUE1)*U2*U5+(-1*U5+VALUE2)*(U4))
      A(NQ,3*GG+1)=-1*((U2*U4+VALUE1)*(-1*U3))
811   CONTINUE
      END IF

      LL1=500
      LL2=501
      LBB=3*GG
      LCC=3*GG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,A)
      DO 999 I=1,3*GG
      BF(I,NN)=A(I,3*GG+1)
999   CONTINUE

      VVU=1/(1+BETA/RAD(1))
      HGD=-1*(BF(1,3)*BF(3,2)-BF(1,2)*BF(3,3))/
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      HGR=-1*(BF(1,1)*BF(3,3)-BF(1,3)*BF(3,1))/
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      XN=NX
      WRITE (*,9)CV,HGD,HGR,XN
      WRITE (25,9)CV,HGD,HGR,XN
3231  CONTINUE
9     FORMAT (5 (F12.6))
      STOP
      END

      SUBROUTINE FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION RAD(2)
      PID=1.D-3
      DTHETA=(PI-4.D0*PID)/(NX-2)
      IF(J==1) THEN
      Z=RAD(I)*DCOS(PID)
      V=RAD(I)*DSIN(PID)
      END IF
      IF((1<J) .AND. (J<=NX/2)) THEN
      Z=RAD(I)*DCOS(PID+(J-1)*DTHETA)
      V=RAD(I)*DSIN(PID+(J-1)*DTHETA)
      END IF
      IF(NX/2<J) THEN
      Z=RAD(I)*DCOS(PI/2.D0+(J-1-NX/2)*DTHETA)
      V=RAD(I)*DSIN(PI/2.D0+(J-1-NX/2)*DTHETA)
      END IF
      U2=Z/RAD(I)
      U3=V/RAD(I)
      R2=RAD(I)
      RETURN
      END
```

```
      SUBROUTINE GAUSL (N,M,II,JJ,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(N,M)
      DO 10 I=1,II
      AA=0.E0
      DO 9 J=1,II
    9 AA=AA+ABS(A(I,J))
      DO 10 J=1,JJ
   10 A(I,J)=A(I,J)/AA
      CALL XXXXX (N,M,II,JJ-II,A)
      RETURN
      END

      SUBROUTINE XXXXX (ND,NCOL,N,NS,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(ND,NCOL)
      N1=N+1
      NT=N+NS
      IF(N.EQ.1) GO TO 50
      DO 10 I=2,N
      IP=I-1
      I1=IP
      X=ABS(A(I1,I1))
      DO 11 J=I,N
      IF(ABS(A(J,I1)).LT.X) GO TO 11
      X=ABS(A(J,I1))
      IP=J
   11 CONTINUE
      IF(IP.EQ.I1) GO TO 13
      DO 12 J=I1,NT
      X=A(I1,J)
      A(I1,J)=A(IP,J)
   12 A(IP,J)=X
   13 DO 10 J=I,N
      X=A(J,I1)/A(I1,I1)
      DO 10 K=I,NT
   10 A(J,K)=A(J,K)-X*A(I1,K)
   50 DO 20 IP=1,N
      I=N1-IP
      DO 20 K=N1,NT
      A(I,K)=A(I,K)/A(I,I)
      IF(I.EQ.1) GO TO 20
      I1=I-1
      DO 25 J=1,I1
   25 A(J,K)=A(J,K)-A(I,K)*A(J,I)
   20 CONTINUE
      RETURN
      END

      SUBROUTINE FUCK2(U2,N,W1,WW1,WWW1,PW1)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PA(0:600)
      PA(0)=0.D0
      PA(1)=(1.-U2**2)**.5
      PA(2)=3.*U2*(1.-U2**2)**.5
      DO 100 J=1,N+1
      PA(J+1)=((2*J+1)*U2*PA(J)-(J+1)*PA(J-1))/(J)
```

```
100   CONTINUE
      W1=PA(N)
      WW1=PA(N-1)
      WWW1=PA(N+1)
      PW1=(N*U2*PA(N)-(N+1)*PA(N-1))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK1(U2,N,W,WW,WWW)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PR(0:550)
      PR(0)=1.D0
      PR(1)=U2
      DO 34 I=2,N+1
      PR(I)=((2*I-1)*U2*PR(I-1)-(I-1)*PR(I-2))/I
34    CONTINUE
      W=PR(N)
      WW=PR(N-1)
      WWW=PR(N+1)
      RETURN
      END

      SUBROUTINE FUCK3(U2,N,W2,WW2,WWW2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PA(0:600)
      PA(0)=0.D0
      PA(1)=0.D0
      PA(2)=3.*(1.-U2**2)
      DO 150 K=2,N+1
      PA(K+1)=((2*K+1)*U2*PA(K)-(K+2)*PA(K-1))/(K-1)
150   CONTINUE
      W2=PA(N)
      WW2=PA(N-1)
      WWW2=PA(N+1)
      RETURN
      END

      SUBROUTINE XXD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SUM1,SUM2,SUM3
     &,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AAN(96),RAD(2)
      DIMENSION AAN1(96),AAN6(96),AAN7(96)
      DIMENSION AAN2(96),AAN5(96),AAN8(96)
      DIMENSION AAN3(96),AAN4(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      B1=AJ0*XX**2.+(YY**2.-XX**2.)*AJ1/DK
      B2=(AJ0-2.*AJ1/DK)/DK**2.
      G5E=DEXP(-1.*E3)
      G6DE=-1.*E3*DEXP(-1.*E3)
      G1DE=-1.*E3*DEXP(-1.*E3)
```

```
  G2DE=E3*DEXP(-1.*E3)
  G3DE=(1.-E3)*DEXP(-1.*E3)
  G4DE=(1.+E3)*DEXP(-1.*E3)
  CALL BEST(N,1,1,0,DKK,-BB,V1)
  CALL BEST(N,1,2,1,DKK,-BB,V2)
  CALL BEST(N-1,2,2,3,DKK,-BB,V3)
  CALL BEST(N-1,0,0,1,DKK,-BB,V4)
  CALL BEST(N-1,2,2,1,DKK,-BB,V9)
  CALL BEST(N-1,1,1,0,DKK,-BB,V11)
  H1B=-N*(2*N-1)*((-BB)**2.)*AJ0*V1+N*(2*N-1)*((-BB)**2.)*B1*V2/
&DK1**2.-.5*(N-2)*(YY**2.-XX**2.)*B2*V3+.5*N*(N+1)*(N-2)*AJ0*V4
  H2B=(-N*(2*N-1)*((-BB)**2.)*(V1-V2)+.5*(N-2)*((-BB)**2.)
&*V9+.5*N*(N+1)*(N-2)*V4)*B1/DK1**2.
  H3B=(DKK*(-BB)**2.)*(-N*(2*N-1)*(-BB)*V1+(N+1)*(N-2)*V11)*B1/
& DK1**2.
  AAN(II)=WET(II)*(G5E*H1B+G6DE*H2B+G1DE*H3B)*DEXP(DDK(II))
  CALL BEST(N+1,2,2,3,DKK,-BB,S1)
  CALL BEST(N+1,0,0,1,DKK,-BB,S2)
  CALL BEST(N+1,2,2,1,DKK,-BB,S5)
  CALL BEST(N+1,0,0,1,DKK,-BB,S6)
  CALL BEST(N+1,1,1,0,DKK,-BB,S9)
  H4B=.5*((YY**2.-XX**2.)*B2*S1-N*(N+1)*AJ0*S2)
  H5B=-.5*(((-BB)**2.)*S5+N*(N+1)*S6)*B1/DK1**2.
  H6B=N*DKK*((-BB)**2.)*B1*S9/DK1**2.
  AAN1(II)=WET(II)*(G5E*H4B+G6DE*H5B+G1DE*H6B)*DEXP(DDK(II))
  CALL BEST(N,2,2,3,DKK,-BB,F1)
  CALL BEST(N,0,0,1,DKK,-BB,F2)
  CALL BEST(N,2,2,1,DKK,-BB,F5)
  CALL BEST(N,0,0,1,DKK,-BB,F6)
  CALL BEST(N,1,1,0,DKK,-BB,F9)
  H7B=-.5*((YY**2.-XX**2.)*B2*F1+N*(N+1)*AJ0*F2)
  H8B=.5*(((-BB)**2.)*F5-N*(N+1)*F6)*B1/DK1**2.
  H9B=DKK*((-BB)**2.)*B1*F9/DK1**2.
  AAN2(II)=WET(II)*(G5E*H7B+G6DE*H8B+G1DE*H9B)*DEXP(DDK(II))
  CALL BEST(N,1,1,2,DKK,-BB,Z1)
  CALL BEST(N-1,2,2,3,DKK,-BB,Z2)
  CALL BEST(N-1,0,0,3,DKK,-BB,Z3)
  CALL BEST(N,1,2,3,DKK,-BB,Z7)
  CALL BEST(N-1,1,1,2,DKK,-BB,Z9)
  H10B=XX*YY*B2*(-N*(2*N-1)*Z1-.5*(N-2)*Z2+N*(N+1)*(N-2)*Z3/2./
&(-BB)**2.)
  H11B=XX*YY*B2*(N*(2*N-1)*Z7+(N-2)*Z2)
  H12B=DKK*XX*YY*B2*(-N*(2*N-1)*(-BB)*Z1+(N+1)*(N-2)*Z9)
  AAN3(II)=WET(II)*(G6DE*H10B+G3DE*H11B+G1DE*H12B)*DEXP(DDK(II))
  CALL BEST(N+1,2,2,3,DKK,-BB,C1)
  CALL BEST(N+1,0,0,3,DKK,-BB,C2)
  CALL BEST(N+1,1,1,2,DKK,-BB,C3)
  H13B=.5*XX*YY*B2*(C1-N*(N+1)*C2/(-BB)**2.)
  H14B=-1.*XX*YY*B2*C1
  H15B=N*DKK*XX*YY*B2*C3
  AAN4(II)=WET(II)*(G6DE*H13B+G3DE*H14B+G1DE*H15B)*DEXP(DDK(II))
  CALL BEST(N,2,2,3,DKK,-BB,Q1)
  CALL BEST(N,0,0,3,DKK,-BB,Q2)
  CALL BEST(N,1,1,2,DKK,-BB,Q3)
  H16B=-.5*XX*YY*B2*(Q1+N*(N+1)*Q2/(-BB)**2.)
  H17B=XX*YY*B2*Q1
  H18B=DKK*XX*YY*B2*Q3
  AAN5(II)=WET(II)*(G6DE*H16B+G3DE*H17B+G1DE*H18B)*DEXP(DDK(II))
```

```
      CALL BEST(N,1,1,2,DKK,-BB,Y1)
      CALL BEST(N,1,2,3,DKK,-BB,Y2)
      CALL BEST(N-1,2,2,3,DKK,-BB,Y3)
      CALL BEST(N-1,0,0,3,DKK,-BB,Y4)
      CALL BEST(N-1,1,1,2,DKK,-BB,Y9)
      H19B=-1.*XX*AJ1*(N*(2*N-1)*(Y1-Y2)-.5*(N-2)*Y3-.5*N*(N+1)*(N-2)*
     &Y4/(-BB)**2.)/DKK**2./DK1
      H20B=-1.*XX*AJ1*(N*(2*N-1)*(-BB)*Y1-(N+1)*(N-2)*Y9)/DK1/DKK
      AAN6(II)=WET(II)*(G2DE*H19B+G4DE*H20B)*DEXP(DDK(II))
      CALL BEST(N+1,2,2,3,DKK,-BB,UU1)
      CALL BEST(N+1,0,0,3,DKK,-BB,UU2)
      CALL BEST(N+1,1,1,2,DKK,-BB,UU3)
      H21B=-.5*XX*AJ1*(UU1+N*(N+1)*UU2/(-BB)**2.)/DKK**2./DK1
      H22B=N*XX*AJ1*UU3/DK1/DKK
      AAN7(II)=WET(II)*(G2DE*H21B+G4DE*H22B)*DEXP(DDK(II))
      CALL BEST(N,2,2,3,DKK,-BB,AW1)
      CALL BEST(N,0,0,3,DKK,-BB,AW2)
      CALL BEST(N,1,1,2,DKK,-BB,AW3)
      H23B=.5*XX*AJ1*(AW1-N*(N+1)*AW2/(-BB)**2.)/DKK**2./DK1
      H24B=XX*AJ1*AW3/DK1/DKK
      AAN8(II)=WET(II)*(G2DE*H23B+G4DE*H24B)*DEXP(DDK(II))
2001  CONTINUE
      SUM1=0.D0
      SUM2=0.D0
      SUM3=0.D0
      SUM4=0.D0
      SUM5=0.D0
      SUM6=0.D0
      SUM7=0.D0
      SUM8=0.D0
      SUM9=0.D0
      DO 1999 IJ=1,IN
      SUM1=SUM1+AAN(IJ)
      SUM2=SUM2+AAN1(IJ)
      SUM3=SUM3+AAN2(IJ)
      SUM4=SUM4+AAN3(IJ)
      SUM5=SUM5+AAN4(IJ)
      SUM6=SUM6+AAN5(IJ)
      SUM7=SUM7+AAN6(IJ)
      SUM8=SUM8+AAN7(IJ)
      SUM9=SUM9+AAN8(IJ)
1999  CONTINUE
      RETURN
      END
      SUBROUTINE BEST(N,M,J,L,ABK,ZZ1,BBB)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PI=DACOS(-1.D0)
      FFD=0.D0
      DO 104 IQ=0,N/2
      CALL GAMMA(N-2*IQ-M,AA1)
      CALL GAMMA(IQ,AA2)
      XZ=ABK*ABS(ZZ1)
      CALL AKV(N,IQ,J,XZ,WK)
      FFD1=((2/PI)**.5)/((-2.D0)**IQ)/AA2/AA1/(ZZ1)**(N+M)
      IF (N-2*IQ-M .LT. 0) THEN
      FFD1=0.D0
      END IF
      FFD=FFD+FFD1*WK*(ABK*ABS(ZZ1))**(N-IQ+L-.5)
```

```
104    CONTINUE
       BBB=FFD
       IF (N .LT. M) THEN
       BBB=0.D0
       END IF
       RETURN
       END

        SUBROUTINE AKV(N,IQ,J,X,FDK)
        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
        DIMENSION AAK(-20:80),FFK(-20:80)
        IF (N-IQ-J .GE. 1) THEN
        NN=N-IQ-J-1
        ELSE
        NN=N-IQ-J
        END IF
        PI=DACOS(-1.D0)
        AAK(0)=-1.*(.5D0*PI/X)/DEXP(X)
        AAK(1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
        AAK(2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
        AAK(-1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
        AAK(-2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
        FFK(0)=(.5D0*PI/X)**.5/DEXP(X)
        FFK(1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
        FFK(2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
        FFK(-1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
        FFK(-2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
        IF (IABS(NN) .LE. 2 ) THEN
        GO TO 2233
        END IF
        DO 502 I=3,IABS(NN)
        AAK(I)=AAK(I-2)-(2*I-1)*AAK(I-1)/X
        FFK(I)=AAK(I)/(-1.)**(I+1)/(.5*PI/X)**.5
        FFK(-I)=FFK(I)
502     CONTINUE
2233    CONTINUE
        FDK=FFK(NN)
4443    CONTINUE
        RETURN
        END

        SUBROUTINE GAMMA(J,AJK)
        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
        IF (J .LE. 0) THEN
        AJK=1.D0
        ELSE
        AJK=1.D0
        DO 300 I=1,J
        SS=DBLE(I)
        AJK=AJK*SS
300     CONTINUE
          END IF
          RETURN
          END

       SUBROUTINE BESSEL(CX,AJ,AJ0,AJ1,AJ2)
       IMPLICIT DOUBLE PRECISION (A-H,O-Z)
       AJ0=0.D0
```

```
      AJ1=0.D0
      AJ2=0.D0
      DO 100 J=0,80
      CALL GAMMA(J,AJK)
      TJ=AJ0
      AJ0=AJ0+((-1.D0)**J)*(CX/2.)**(2*J)/(AJK)**2.
      IF (ABS(AJ0-TJ) .LE. 0.000000000000001 ) THEN
      GO TO    500
      END IF
100   CONTINUE
500   CONTINUE
      DO 107 J=0,80
      CALL GAMMA(J,AJK)
      TJ1=AJ1
      AJ1=AJ1+((-1.D0)**J)*(CX/2.)**(2*J+1)/((AJK)**2.)/(J+1)
      IF (ABS(AJ1-TJ1) .LE. 0.000000000000001 ) THEN
      GO TO 201
      END IF
107   CONTINUE
201   CONTINUE
      DO 108 J=0,80
      CALL GAMMA(J,AJK)
      TJ2=AJ2
      AJ2=AJ2+((-1.D0)**J)*(CX/2.)**(2*J+2)/((AJK)**2.)/(J+1)
     &/(J+2)
      IF (ABS(AJ2-TJ2)    .LE. 0.0000000000000001) THEN
      GO TO 200
        END IF
108   CONTINUE
200   CONTINUE
        AJ=-1.*AJ1
        RETURN
        END

      SUBROUTINE XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3,SM4)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN4(96),RAD(2),AN1(96),AN2(96),AN3(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=-1.D0*DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      DK2=DKK*RAD(1)*U2
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      PAJ0=-AJ1
      AJ3=4*AJ2/DK-AJ1
      PPAJ1=(-3*AJ1/4+AJ3/4)
      CALL BEST(N+1,1,1,0,DKK,-BB,VV1)
      AN1(II)=WET(II)*N*(
     &DKK*(-BB)**2.*U2*DEXP(E3)*AJ1*VV1*U4-DKK*(-BB)**2.*U3
     &*DEXP(E3)*PAJ1*VV1*U4)*DEXP(DKK)
      AN2(II)=WET(II)*N*((DKK*U3)**2.*(
     &-(-BB)**2.*DEXP(E3)*PPAJ1*VV1*U4)
     &+2*(PAJ1*DKK*U3*(
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```
     &+DKK*(-BB)**2.*U2*DEXP(E3)*VV1*U4))
     &+AJ1*(DKK*U2)**2*(
     &-(-BB)**2.*DEXP(E3)*VV1*U4))*DEXP(DKK)
      AN3(II)=WET(II)*N*(
     &-DKK*(-BB)**2.*RAD(1)*U3*DEXP(E3)*AJ1*VV1*U4-
     &DKK*(-BB)**2.*RAD(1)*U2*DEXP(E3)*PAJ1*VV1*U4)*
     &DEXP(DKK)
      AN4(II)=WET(II)*N*(-1*U5)*(
     &-1.D0*(-BB)**2.*AJ1*VV1*DEXP(E3))*DEXP(DKK)
2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      SM4=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN1(IJ)
      SM2=SM2+AN2(IJ)
      SM3=SM3+AN3(IJ)
      SM4=SM4+AN4(IJ)
1999  CONTINUE
      RETURN
      END




CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                 FOR LINEAR CONCENTRATION PROFILE                        C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


      SUBROUTINE XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3,SM4)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN4(96),RAD(2),AN1(96),AN2(96),AN3(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=-1.D0*DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      DK2=DKK*RAD(1)*U2
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      PAJ0=-AJ1
      AJ3=4*AJ2/DK-AJ1
      PPAJ1=(-3*AJ1/4+AJ3/4)
      CALL BEST(N+1,1,1,0,DKK,-BB,VV1)
      AN1(II)=WET(II)*N*(
     &DKK*(-BB)**2.*U2*DEXP(E3)*AJ1*VV1*U4-DKK*(-BB)**2.*U3
     &*DEXP(E3)*PAJ1*VV1*U4)*DEXP(DKK)
      AN2(II)=WET(II)*N*
     &((DKK*U3)**2.*(
     &-(-BB)**2.*DEXP(E3)*PPAJ1*VV1*U4)
     &+2*(PAJ1*DKK*U3*(
```

```
     &+DKK*(-BB)**2.*U2*DEXP(E3)*VV1*U4))
     &+AJ1*(DKK*U2)**2*(
     &-(-BB)**2.*DEXP(E3)*VV1*U4))*DEXP(DKK)
      AN3(II)=WET(II)*N*(
     &-DKK*(-BB)**2.*RAD(1)*U3*DEXP(E3)*AJ1*VV1*U4-
     &DKK*(-BB)**2.*RAD(1)*U2*DEXP(E3)*PAJ1*VV1*U4)*
     &DEXP(DKK)
      AN4(II)=WET(II)*N*(-1*U5)*(
     &-1.D0*(-BB)**2.*AJ1*VV1*DEXP(E3))*DEXP(DKK)
2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      SM4=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN1(IJ)
      SM2=SM2+AN2(IJ)
      SM3=SM3+AN3(IJ)
      SM4=SM4+AN4(IJ)
1999  CONTINUE
      RETURN
      END
```

Appendix E1-2: Computer programming source code for estimating the diffusio-phoretic velocity of single spherical particle parallel two solute impenetrable plates.

```
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(500,501),RAD(2),DDK(96),WET(96),B(500,501), BF(500,3)
      INTEGER GGG,T,GG,NX,LL1,LL2,LBB,LCC
      OPEN (23,FILE='GAUSS80.DAT',STATUS='OLD')
      OPEN (25,FILE='DD-10.TXT',STATUS='NEW')
      OPEN (24,FILE='WET3.DAT',STATUS='OLD')
      IN=80
      BB=0.1D0
      TR=1.D0
      CC=BB*TR
      DO 1001 I=1,IN
      READ (23,*) DDK(I),WET(I)
1001  CONTINUE
      T=1
      PI=DACOS(-1.D0)
      FI=.01*PI/180.
      U4=DCOS(FI)
      U5=DSIN(FI)
      DO 3231 IUY=1,50
      READ (24,*) CV,NX
      RAD(1)=CV*BB
      BETA=10.D0*RAD(1)
      GGG=NX
      DO 511 I=1,T
      DO 512 J=1,NX
      NU=J
      DO 513 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      B(NU,GGG+1)=-1*(1-BETA*2/R2)*(U3*U4)
      DO 514 N=1,NX
      NZ=N
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3,SM4)
      B(NU,NZ)=(1-BETA*2/R2)*((-N-1)*R2**(-1*(N+2))*W1*U4+SM1)
     &-BETA*((N+1)*(N+2)*R2**(-1*(N+3))*W1*U4+SM2)
 514  CONTINUE
 513  CONTINUE
 512  CONTINUE
 511  CONTINUE
      LL1=500
      LL2=501
      LBB=GGG
      LCC=GGG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,B)
```

```
      GG=T*NX
      DO 7765 NN=1,3
      DO 111 I=1,T
      DO 112 J=1,NX
      NO=J+NX*(I-1)
      NP=J+NX*(I-1)+T*NX
      NQ=J+NX*(I-1)+2*T*NX
      DO 113 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      IF(NN .EQ. 1) THEN
      A(NO,3*GG+1)=1.D0
      A(NP,3*GG+1)=0.D0
      A(NQ,3*GG+1)=0.D0
      END IF

      IF(NN .EQ. 2) THEN
      A(NO,3*GG+1)=U2
      A(NP,3*GG+1)=0.D0
      A(NQ,3*GG+1)=-1*U3*U4
      END IF

      DO 114 N=1,NX
      NE=(3*N-2)+3*NX*(K-1)
      NF=(3*N-1)+3*NX*(K-1)
      NG=(3*N-0)+3*NX*(K-1)

      CALL FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
      CALL XXD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,
     &WET,SUM1,SUM2,SUM3,SUM4,
     &SUM5,SUM6,SUM7,SUM8,SUM9)
      A(NO,NE)=((2.*N*(2*N-1)*U3*W1*U4**2.+(N-2)*WW2*DCOS(2.*FI)-
     &N*(N+1)*(N-2)*WW)/2./R2**(N))+SUM1
      A(NO,NF)=(-1.*(WWW2*DCOS(2.*FI)-
     &N*(N+1)*WWW)/2./R2**(N+2)+SUM2)
      A(NO,NG)=((W2*DCOS(2.*FI)+N*(N+1)*W)/2./R2**(N+1)+SUM3)
      A(NP,NE)=(N*(2*N-1)*U3*W1+(N-2)*WW2)*U4*U5/R2**(N)+SUM4
      A(NP,NF)=-(WWW2*U4*U5)/R2**(N+2)+SUM5
      A(NP,NG)=(W2*U4*U5)/R2**(N+1)+SUM6
      A(NQ,NE)=((N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U4/R2**N+SUM7)
      A(NQ,NF)=(-(N*WWW1*U4)/R2**(N+2)+SUM8)
      A(NQ,NG)=(-(W1*U4)/R2**(N+1)+SUM9)
114   CONTINUE
113   CONTINUE
112   CONTINUE
111   CONTINUE
```

```
      IF(NN .EQ. 3) THEN
      DO 811 J=1,NX
      NO=J
      NP=J+NX
      NQ=J+2*NX
      CALL FU(1,J,1,NX,RAD,PI,U2,U3,R2)
      VALUE1=0.D0
      VALUE2=0.D0
      DO 713 KK=1,NX
      NZ=KK
      CALL FUCK2(U2,KK,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL XRD(KK,BB,CC,IN,RAD,U2,U3,U4,U5,
     &DDK,WET,SM1,SM2,SM3,SM4)
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      VALUE1=VALUE1
     &+B(NZ,GGG+1)*(-1*RAD(1)**(-KK-2)*PW1*U3*U4+SM3/RAD(1))
      VALUE2=VALUE2
     &+B(NZ,GGG+1)*(-1*RAD(1)**(-KK-2)*W1*U5/U3+SM4/(RAD(1)*U3))
713   CONTINUE
      A(NO,3*GG+1)=-1*((U2*U4+VALUE1)*U2*U4+(-1*U5+VALUE2)*(-1*U5))
      A(NP,3*GG+1)=-1*((U2*U4+VALUE1)*U2*U5+(-1*U5+VALUE2)*(U4))
      A(NQ,3*GG+1)=-1*((U2*U4+VALUE1)*(-1*U3))
811   CONTINUE
      END IF
      LL1=500
      LL2=501
      LBB=3*GG
      LCC=3*GG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,A)
      WRITE(*,*) A(1,3*GG+1)
      DO 999 I=1,3*GG
      BF(I,NN)=A(I,3*GG+1)
999   CONTINUE
7765  CONTINUE
      VVU=1/(1+BETA/RAD(1))
      XN=NX
      HGD=-1*(BF(1,3)*BF(3,2)-BF(1,2)*BF(3,3))/
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      HGR=-1*(BF(1,1)*BF(3,3)-BF(1,3)*BF(3,1))/
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      WRITE (*,9)CV,HGD,HGR,XN
      WRITE (25,9)CV,HGD,HGR,XN
3231  CONTINUE
9     FORMAT (5(F12.5))
      STOP
      END
```

```
  SUBROUTINE XXD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,
&SUM1,SUM2,SUM3,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9)
  IMPLICIT DOUBLE PRECISION (A-H,O-Z)
  DIMENSION WET(96),DDK(96),AAN(96),RAD(2)
  DIMENSION AAN1(96),AAN6(96),AAN7(96)
  DIMENSION AAN2(96),AAN5(96),AAN8(96)
  DIMENSION AAN3(96),AAN4(96)

  DO 2001 II=1,IN
  ZZ=RAD(1)*U2
  XX=RAD(1)*U3*U4
  YY=RAD(1)*U3*U5
  E1=DDK(II)*(BB+CC)
  E2=DDK(II)*(ZZ-CC)
  E3=DDK(II)*(ZZ+BB)
  DK=DDK(II)*RAD(1)*U3
  DKK=DDK(II)
  DK1=RAD(1)*U3

  CALL BESSEL(DK,AJ0,AJ1,AJ2)
  B1=AJ0*XX**2.+(YY**2.-XX**2.)*AJ1/DK
  B2=(AJ0-2.*AJ1/DK)/DK**2.
  DETA1=2.D0*DSINH(E1)
  DETA2=4.D0*((DSINH(E1))**2.-E1**2.)
  G5E=(-2.*DSINH(E2))/DETA1
  G5D=(-2.*DSINH(E3))/DETA1
  G6DE=8.*E1**2.*(E3*(DSINH(E1)/E1)*(DSINH(E3)/E3-DSINH(E1)*DCOSH
&(E2)/E1)+E2*(DSINH(E1)*DCOSH(E3)/E1-DSINH(E2)/E2))/DETA1/DETA2
  G6ED=8.*E1**2.*(E2*(DSINH(E1)/E1)*(DSINH(E2)/E2-DSINH(E1)*DCOSH
&(E3)/E1)+E3*(DSINH(E1)*DCOSH(E2)/E1-DSINH(E3)/E3))/DETA1/DETA2
  G1DE=4.*E1*E3*E2*(DSINH(E3)/E3
&+DSINH(E1)*DSINH(E2)/E1/E2)/DETA2
  G1ED=4.*E1*E2*E3*(DSINH(E2)/E2
&+DSINH(E1)*DSINH(E3)/E1/E3)/DETA2
  G2DE=4.*E1*E3*E2*(DSINH(E3)/E3-DSINH(E1)*DSINH(E2)/E1/E2)/DETA2
  G2ED=4.*E1*E2*E3*(DSINH(E2)/E2-DSINH(E1)*DSINH(E3)/E1/E3)/DETA2
  G3DE=4.*E1*(E2*(DCOSH(E3)-
&DSINH(E1)*DSINH(E2)/E1/E2)+E3*(SINH(E3)
&/E3-DSINH(E1)*DCOSH(E2)/E1))/DETA2
  G3ED=4.*E1*(E3*(DCOSH(E2)-
&DSINH(E1)*DSINH(E3)/E1/E3)+E2*(SINH(E2)
&/E2-DSINH(E1)*DCOSH(E3)/E1))/DETA2
  G4DE=4.*E1*(E2*(DCOSH(E3)-DSINH(E1)*DSINH(E2)/E1/E2)-
&E3*(SINH(E3)/E3-DSINH(E1)*DCOSH(E2)/E1))/DETA2
  G4ED=4.*E1*(E3*(DCOSH(E2)-DSINH(E1)*DSINH(E3)/E1/E3)-
&E2*(SINH(E2)/E2-DSINH(E1)*DCOSH(E3)/E1))/DETA2

  CALL BEST(N,1,1,0,DKK,-BB,V1)
  CALL BEST(N,1,2,1,DKK,-BB,V2)
```

```
  CALL BEST(N-1,2,2,3,DKK,-BB,V3)
  CALL BEST(N-1,0,0,1,DKK,-BB,V4)
  CALL BEST(N,1,1,0,DKK,CC,V5)
  CALL BEST(N,1,2,1,DKK,CC,V6)
  CALL BEST(N-1,2,2,3,DKK,CC,V7)
  CALL BEST(N-1,0,0,1,DKK,CC,V8)
  CALL BEST(N-1,2,2,1,DKK,-BB,V9)
  CALL BEST(N-1,2,2,1,DKK,CC,V10)
  CALL BEST(N-1,1,1,0,DKK,-BB,V11)
  CALL BEST(N-1,1,1,0,DKK,CC,V12)

  H1B=-N*(2*N-1)*((-BB)**2.)*AJ0*V1+N*(2*N-1)*((-BB)**2.)*B1*V2/
&DK1**2.-.5*(N-2)*(YY**2.-XX**2.)*B2*V3+.5*N*(N+1)*(N-2)*AJ0*V4
  H1C=-N*(2*N-1)*(CC**2.)*AJ0*V5+N*(2*N-1)*(CC**2.)*B1*V6/
&DK1**2.-.5*(N-2)*(YY**2.-XX**2.)*B2*V7+.5*N*(N+1)*(N-2)*AJ0*V8
  H2B=(-N*(2*N-1)*((-BB)**2.)*(V1-V2)+.5*(N-2)*((-BB)**2.)
&*V9+.5*N*(N+1)*(N-2)*V4)*B1/DK1**2.
  H2C=(-N*(2*N-1)*(CC**2.)*(V5-V6)+.5*(N-2)*(CC**2.) *V10
&+.5*N*(N+1)*(N-2)*V8)*B1/DK1**2.
  H3B=(DKK*(-BB)**2.)*(-N*(2*N-1)*(-BB)*V1+(N+1)*(N-2)*V11)*B1/
&DK1**2.
  H3C=(DKK*CC**2.)*(-N*(2*N-1)*CC*V5+(N+1)*(N-2)*V12)*B1/DK1**2.
  AAN(II)=WET(II)*(G5E*H1B-G5D*H1C+G6DE*H2B-
&G6ED*H2C+G1DE*H3B-G1ED*H3C)*DEXP(DDK(II))

  CALL BEST(N+1,2,2,3,DKK,-BB,S1)
  CALL BEST(N+1,0,0,1,DKK,-BB,S2)
  CALL BEST(N+1,2,2,3,DKK,CC,S3)
  CALL BEST(N+1,0,0,1,DKK,CC,S4)
  CALL BEST(N+1,2,2,1,DKK,-BB,S5)
  CALL BEST(N+1,0,0,1,DKK,-BB,S6)
  CALL BEST(N+1,2,2,1,DKK,CC,S7)
  CALL BEST(N+1,0,0,1,DKK,CC,S8)
  CALL BEST(N+1,1,1,0,DKK,-BB,S9)
  CALL BEST(N+1,1,1,0,DKK,CC,S10)
  H4B=.5*((YY**2.-XX**2.)*B2*S1-N*(N+1)*AJ0*S2)
  H4C=.5*((YY**2.-XX**2.)*B2*S3-N*(N+1)*AJ0*S4)
  H5B=-.5*(((-BB)**2.)*S5+N*(N+1)*S6)*B1/DK1**2.
  H5C=-.5*((CC**2.)*S7+N*(N+1)*S8)*B1/DK1**2.
  H6B=N*DKK*((-BB)**2.)*B1*S9/DK1**2.
  H6C=N*DKK*(CC**2.)*B1*S10/DK1**2.

  AAN1(II)=WET(II)*(G5E*H4B-G5D*H4C+G6DE*H5B-
&G6ED*H5C+G1DE*H6B-G1ED*
&H6C)*DEXP(DDK(II))

  CALL BEST(N,2,2,3,DKK,-BB,F1)
  CALL BEST(N,0,0,1,DKK,-BB,F2)
  CALL BEST(N,2,2,3,DKK,CC,F3)
```

```
  CALL BEST(N,0,0,1,DKK,CC,F4)
  CALL BEST(N,2,2,1,DKK,-BB,F5)
  CALL BEST(N,0,0,1,DKK,-BB,F6)
  CALL BEST(N,2,2,1,DKK,CC,F7)
  CALL BEST(N,0,0,1,DKK,CC,F8)
  CALL BEST(N,1,1,0,DKK,-BB,F9)
  CALL BEST(N,1,1,0,DKK,CC,F10)

  H7B=-.5*((YY**2.-XX**2.)*B2*F1+N*(N+1)*AJ0*F2)
  H7C=-.5*((YY**2.-XX**2.)*B2*F3+N*(N+1)*AJ0*F4)
  H8B=.5*(((-BB)**2.)*F5-N*(N+1)*F6)*B1/DK1**2.
  H8C=.5*((CC**2.)*F7-N*(N+1)*F8)*B1/DK1**2.
  H9B=DKK*((-BB)**2.)*B1*F9/DK1**2.
  H9C=DKK*(CC**2.)*B1*F10/DK1**2.

  AAN2(II)=WET(II)*(G5E*H7B-G5D*H7C+G6DE*H8B-
&G6ED*H8C+G1DE*H9B-G1ED*H9C)*DEXP(DDK(II))

  CALL BEST(N,1,1,2,DKK,-BB,Z1)
  CALL BEST(N-1,2,2,3,DKK,-BB,Z2)
  CALL BEST(N-1,0,0,3,DKK,-BB,Z3)
  CALL BEST(N,1,1,2,DKK,CC,Z4)
  CALL BEST(N-1,2,2,3,DKK,CC,Z5)
  CALL BEST(N-1,0,0,3,DKK,CC,Z6)
  CALL BEST(N,1,2,3,DKK,-BB,Z7)
  CALL BEST(N,1,2,3,DKK,CC,Z8)
  CALL BEST(N-1,1,1,2,DKK,-BB,Z9)
  CALL BEST(N-1,1,1,2,DKK,CC,Z10)
  H10B=XX*YY*B2*(-N*(2*N-1)*Z1-.5*(N-2)*Z2+N*(N+1)*(N-2)*Z3/2./
&(-BB)**2.)
  H10C=XX*YY*B2*(-N*(2*N-1)*Z4-.5*(N-2)*Z5+N*(N+1)*(N-2)*Z6/2/
&CC**2.)
  H11B=XX*YY*B2*(N*(2*N-1)*Z7+(N-2)*Z2)
  H11C=XX*YY*B2*(N*(2*N-1)*Z8+(N-2)*Z5)
  H12B=DKK*XX*YY*B2*(-N*(2*N-1)*(-BB)*Z1+(N+1)*(N-2)*Z9)
  H12C=DKK*XX*YY*B2*(-N*(2*N-1)*CC*Z4+(N+1)*(N-2)*Z10)
  AAN3(II)=WET(II)*(G6DE*H10B-G6ED*H10C+G3DE*H11B-
&G3ED*H11C+G1DE*H12B-G1ED*H12C)*DEXP(DDK(II))
  CALL BEST(N+1,2,2,3,DKK,-BB,C1)
  CALL BEST(N+1,0,0,3,DKK,-BB,C2)
  CALL BEST(N+1,1,1,2,DKK,-BB,C3)
  CALL BEST(N+1,2,2,3,DKK,CC,C4)
  CALL BEST(N+1,0,0,3,DKK,CC,C5)
  CALL BEST(N+1,1,1,2,DKK,CC,C6)
  H13B=.5*XX*YY*B2*(C1-N*(N+1)*C2/(-BB)**2.)
  H13C=.5*XX*YY*B2*(C4-N*(N+1)*C5/CC**2.)
  H14B=-1.*XX*YY*B2*C1
  H14C=-1.*XX*YY*B2*C4
  H15B=N*DKK*XX*YY*B2*C3
```

```
  H15C=N*DKK*XX*YY*B2*C6

  AAN4(II)=WET(II)*(G6DE*H13B-G6ED*H13C+G3DE*H14B-
&G3ED*H14C+G1DE*H15B-G1ED*H15C)*DEXP(DDK(II))

  CALL BEST(N,2,2,3,DKK,-BB,Q1)
  CALL BEST(N,0,0,3,DKK,-BB,Q2)
  CALL BEST(N,1,1,2,DKK,-BB,Q3)
  CALL BEST(N,2,2,3,DKK,CC,Q4)
  CALL BEST(N,0,0,3,DKK,CC,Q5)
  CALL BEST(N,1,1,2,DKK,CC,Q6)

  H16B=-.5*XX*YY*B2*(Q1+N*(N+1)*Q2/(-BB)**2.)
  H16C=-.5*XX*YY*B2*(Q4+N*(N+1)*Q5/CC**2.)
  H17B=XX*YY*B2*Q1
  H17C=XX*YY*B2*Q4
  H18B=DKK*XX*YY*B2*Q3
  H18C=DKK*XX*YY*B2*Q6

  AAN5(II)=WET(II)*(G6DE*H16B-G6ED*H16C+G3DE*H17B-
&G3ED*H17C+G1DE*H18B-G1ED*H18C)*DEXP(DDK(II))

  CALL BEST(N,1,1,2,DKK,-BB,Y1)
  CALL BEST(N,1,2,3,DKK,-BB,Y2)
  CALL BEST(N-1,2,2,3,DKK,-BB,Y3)
  CALL BEST(N-1,0,0,3,DKK,-BB,Y4)
  CALL BEST(N,1,1,2,DKK,CC,Y5)
  CALL BEST(N,1,2,3,DKK,CC,Y6)
  CALL BEST(N-1,2,2,3,DKK,CC,Y7)
  CALL BEST(N-1,0,0,3,DKK,CC,Y8)
  CALL BEST(N-1,1,1,2,DKK,-BB,Y9)
  CALL BEST(N-1,1,1,2,DKK,CC,Y10)

  H19B=-1.*XX*AJ1*(N*(2*N-1)*(Y1-Y2)-.5*(N-2)*Y3-.5*N*(N+1)*(N-2)*
& Y4/(-BB)**2.)/DKK**2./DK1
  H19C=-1.*XX*AJ1*(N*(2*N-1)*(Y5-Y6)-.5*(N-2)*Y7-.5*N*(N+1)*(N-2)*
& Y8/CC**2.)/DKK**2./DK1
  H20B=-1.*XX*AJ1*(N*(2*N-1)*(-BB)*Y1-(N+1)*(N-2)*Y9)/DK1/DKK
  H20C=-1.*XX*AJ1*(N*(2*N-1)*CC*Y5-(N+1)*(N-2)*Y10)/DK1/DKK

  AAN6(II)=WET(II)*(G2DE*H19B-G2ED*H19C+G4DE*H20B-G4ED*H20C)
&*DEXP(DDK(II))

  CALL BEST(N+1,2,2,3,DKK,-BB,UU1)
  CALL BEST(N+1,0,0,3,DKK,-BB,UU2)
  CALL BEST(N+1,1,1,2,DKK,-BB,UU3)
  CALL BEST(N+1,2,2,3,DKK,CC,UU4)
  CALL BEST(N+1,0,0,3,DKK,CC,UU5)
  CALL BEST(N+1,1,1,2,DKK,CC,UU6)
```

```
      H21B=-.5*XX*AJ1*(UU1+N*(N+1)*UU2/(-BB)**2.)/DKK**2./DK1
      H21C=-.5*XX*AJ1*(UU4+N*(N+1)*UU5/CC**2.)/DKK**2./DK1
      H22B=N*XX*AJ1*UU3/DK1/DKK
      H22C=N*XX*AJ1*UU6/DK1/DKK

      AAN7(II)=WET(II)*(G2DE*H21B-G2ED*H21C+G4DE*H22B-G4ED*H22C)
     &*DEXP(DDK(II))

      CALL BEST(N,2,2,3,DKK,-BB,AW1)
      CALL BEST(N,0,0,3,DKK,-BB,AW2)
      CALL BEST(N,1,1,2,DKK,-BB,AW3)
      CALL BEST(N,2,2,3,DKK,CC,AW4)
      CALL BEST(N,0,0,3,DKK,CC,AW5)
      CALL BEST(N,1,1,2,DKK,CC,AW6)

      H23B=.5*XX*AJ1*(AW1-N*(N+1)*AW2/(-BB)**2.)/DKK**2./DK1
      H23C=.5*XX*AJ1*(AW4-N*(N+1)*AW5/CC**2.)/DKK**2./DK1
      H24B=XX*AJ1*AW3/DK1/DKK
      H24C=XX*AJ1*AW6/DK1/DKK

      AAN8(II)=WET(II)*(G2DE*H23B-G2ED*H23C+G4DE*H24B-G4ED*H24C)
     &*DEXP(DDK(II))

2001  CONTINUE
      SUM1=0.D0
      SUM2=0.D0
      SUM3=0.D0
      SUM4=0.D0
      SUM5=0.D0
      SUM6=0.D0
      SUM7=0.D0
      SUM8=0.D0
      SUM9=0.D0
      DO 1999 IJ=1,IN
      SUM1=SUM1+AAN(IJ)
      SUM2=SUM2+AAN1(IJ)
      SUM3=SUM3+AAN2(IJ)
      SUM4=SUM4+AAN3(IJ)
      SUM5=SUM5+AAN4(IJ)
      SUM6=SUM6+AAN5(IJ)
      SUM7=SUM7+AAN6(IJ)
      SUM8=SUM8+AAN7(IJ)
      SUM9=SUM9+AAN8(IJ)
1999  CONTINUE
      RETURN
      END

      SUBROUTINE BEST(N,M,J,L,ABK,ZZ1,BBB)
```

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PI=DACOS(-1.D0)
      FFD=0.D0
      DO 104 IQ=0,N/2
      CALL GAMMA(N-2*IQ-M,AA1)
      CALL GAMMA(IQ,AA2)
      XZ=ABK*ABS(ZZ1)
      CALL AKV(N,IQ,J,XZ,WK)
      FFD1=((2/PI)**.5)/((-2.D0)**IQ)/AA2/AA1/(ZZ1)**(N+M)
      IF (N-2*IQ-M .LT. 0) THEN
      FFD1=0.D0
      END IF
      FFD=FFD+FFD1*WK*(ABK*ABS(ZZ1))**(N-IQ+L-.5)
104   CONTINUE
      BBB=FFD
      IF (N .LT. M) THEN
      BBB=0.D0
      END IF
      RETURN
      END

      SUBROUTINE AKV(N,IQ,J,X,FDK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION AAK(-20:80),FFK(-20:80)
      IF (N-IQ-J .GE. 1) THEN
      NN=N-IQ-J-1
      ELSE
      NN=N-IQ-J
      END IF
      PI=DACOS(-1.D0)
      AAK(0)=-1.*(.5D0*PI/X)/DEXP(X)
      AAK(1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      AAK(-1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(-2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(0)=(.5D0*PI/X)**.5/DEXP(X)
      FFK(1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(-1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(-2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      IF (IABS(NN) .LE. 2 ) THEN
      GO TO 2233
      END IF
      DO 502 I=3,IABS(NN)
      AAK(I)=AAK(I-2)-(2*I-1)*AAK(I-1)/X
      FFK(I)=AAK(I)/(-1.)**(I+1)/(.5*PI/X)**.5
      FFK(-I)=FFK(I)
502   CONTINUE
2233  CONTINUE
```

```
      FDK=FFK(NN)
4443  CONTINUE
      RETURN
      END

      SUBROUTINE GAMMA(J,AJK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IF (J .LE. 0) THEN
      AJK=1.D0
      ELSE
      AJK=1.D0
      DO 300 I=1,J
      SS=DBLE(I)
      AJK=AJK*SS
300   CONTINUE
      END IF
      RETURN
      END

      SUBROUTINE BESSEL(X,AJ0,AJ1,AJ2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      AJ0=0.D0
      AJ1=0.D0
      AJ2=0.D0
      DO 100 J=0,50
      CALL GAMMA(J,AJK)
      TJ=AJ0
      AJ0=AJ0+((-1.D0)**J)*(X/2)**(2*J)/(AJK)**2.
      IF (ABS(AJ0-TJ) .LE. 0.000000000000001 ) THEN
      GOTO    500
      END IF
100   CONTINUE
500   CONTINUE
      DO 107 J=0,50
      CALL GAMMA(J,AJK)
      TJ1=AJ1
      AJ1=AJ1+((-1.D0)**J)*(X/2)**(2*J+1)/((AJK)**2.)/(J+1)
      IF (ABS(AJ1-TJ1) .LE. 0.000000000000001 ) THEN
      GO TO 201
      END IF
107   CONTINUE
201   CONTINUE
      DO 108 J=0,50
      CALL GAMMA(J,AJK)
      TJ2=AJ2
      AJ2=AJ2+((-1.D0)**J)*(X/2.)**(2*J+2)/((AJK)**2.)/(J+1)
     &/(J+2)
      IF (ABS(AJ2-TJ2)    .LE. 0.0000000000000001) THEN
      GO TO 200
```

```
      END IF
108   CONTINUE
200   CONTINUE
      RETURN
      END

      SUBROUTINE FU(I,J,K,X,RAD,PI,U2,U3,R2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION RAD(2)
      INTEGER X
      PID=1.D-3
      DTHETA=(PI-4.D0*PID)/(X-2)
      IF(J==1) THEN
      Z=RAD(I)*DCOS(PID)
      V=RAD(I)*DSIN(PID)
      END IF
      IF((1<J) .AND. (J<=X/2)) THEN
      Z=RAD(I)*DCOS(PID+(J-1)*DTHETA)
      V=RAD(I)*DSIN(PID+(J-1)*DTHETA)
      END IF
      IF(X/2<J) THEN
      Z=RAD(I)*DCOS(PI/2.D0+(J-1-X/2)*DTHETA)
      V=RAD(I)*DSIN(PI/2.D0+(J-1-X/2)*DTHETA)
      END IF
      U2=Z/RAD(I)
      U3=V/RAD(I)
      R2=RAD(I)
      RETURN
      END

      SUBROUTINE GAUSL (N,M,II,JJ,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(N,M)
      DO 10 I=1,II
      AA=0.E0
      DO 9 J=1,II
9     AA=AA+ABS(A(I,J))
      DO 10 J=1,JJ
10    A(I,J)=A(I,J)/AA
      CALL XXXXX (N,M,II,JJ-II,A)
      RETURN
      END

      SUBROUTINE XXXXX (ND,NCOL,N,NS,A)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(ND,NCOL)
      N1=N+1
      NT=N+NS
      IF(N.EQ.1) GO TO 50
```

```
      DO 10 I=2,N
      IP=I-1
      I1=IP
      X=ABS(A(I1,I1))
      DO 11 J=I,N
      IF(ABS(A(J,I1)).LT.X) GO TO 11
      X=ABS(A(J,I1))
      IP=J
11    CONTINUE
      IF(IP.EQ.I1) GO TO 13
      DO 12 J=I1,NT
      X=A(I1,J)
      A(I1,J)=A(IP,J)
12    A(IP,J)=X
13    DO 10 J=I,N
      X=A(J,I1)/A(I1,I1)
      DO 10 K=I,NT
10    A(J,K)=A(J,K)-X*A(I1,K)
50    DO 20 IP=1,N
      I=N1-IP
      DO 20 K=N1,NT
      A(I,K)=A(I,K)/A(I,I)
      IF(I.EQ.1) GO TO 20
      I1=I-1
      DO 25 J=1,I1
25    A(J,K)=A(J,K)-A(I,K)*A(J,I)
20    CONTINUE
      RETURN
      END

      SUBROUTINE FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION PA(-1:600)
      PA(-1)=0.D0
      PA(0)=0.D0
      PA(1)=(1.-U2**2)**.5
      PA(2)=3.*U2*(1.-U2**2)**.5
      DO 100 J=1,N+1
      PA(J+1)=((2*J+1)*U2*PA(J)-(J+1)*PA(J-1))/(J)
 100  CONTINUE
      W1=PA(N)
      WW1=PA(N-1)
      WWW1=PA(N+1)
      PW1=(N*U2*PA(N)-(N+1)*PA(N-1))/(U2**2.-1.)
      PWW1=((N-1)*U2*PA(N-1)-(N)*PA(N-2))/(U2**2.-1.)
      PWWW1=((N+1)*U2*PA(N+1)-(N+2)*PA(N))/(U2**2.-1.)
      RETURN
      END
```

```
      SUBROUTINE FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION PR(-1:600)
      PR(-1)=0.D0
      PR(0)=1.D0
      PR(1)=U2
      DO 34 I=2,N+1
      PR(I)=((2*I-1)*U2*PR(I-1)-(I-1)*PR(I-2))/I
34    CONTINUE
      W=PR(N)
      WW=PR(N-1)
      WWW=PR(N+1)
      PW=(N*U2*PR(N)-N*PR(N-1))/(U2**2.-1.)
      PWW=((N-1)*U2*PR(N-1)-(N-1)*PR(N-2))/(U2**2.-1.)
      PWWW=((N+1)*U2*PR(N+1)-(N+1)*PR(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION PB(-1:600)
      PB(-1)=0.D0
      PB(0)=0.D0
      PB(1)=0.D0
      PB(2)=3.*(1.-U2**2)
      DO 150 K=2,N+1
      PB(K+1)=((2*K+1)*U2*PB(K)-(K+2)*PB(K-1))/(K-1)
150   CONTINUE
      W2=PB(N)
      WW2=PB(N-1)
      WWW2=PB(N+1)
      PW2=(N*U2*PB(N)-(N+2)*PB(N-1))/(U2**2.-1.)
      PWW2=((N-1)*U2*PB(N-1)-(N+1)*PB(N-2))/(U2**2.-1.)
      PWWW2=((N+1)*U2*PB(N+1)-(N+3)*PB(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,
     &DDK,WET,SM1,SM2,SM3,SM4)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN4(96),RAD(2),AN1(96),AN2(96),AN3(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      E2=DDK(II)*(ZZ-CC)
      E1=DDK(II)*(BB+CC)
      DK=DDK(II)*RAD(1)*U3
```

```
      DKK=DDK(II)
      DK1=RAD(1)*U3
      DK2=DKK*RAD(1)*U2
      CALL BESSEL(DK,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      PAJ0=-AJ1
      AJ3=4*AJ2/DK-AJ1
      PPAJ1=(-3*AJ1/4+AJ3/4)
      CALL BEST(N+1,1,1,0,DKK,-BB,VV1)
      CALL BEST (N+1,1,1,0,DKK,CC,VV2)

      AN1(II)=WET(II)*N*(DKK*CC**2.*U2*DSINH(E3)*AJ1*U4*VV2/DSINH(
     & E1)+DKK*CC**2.*U3*DCOSH(E3)*PAJ1*VV2*U4/DSINH(E1)-DKK*
     & (-BB)**2.*U2*DSINH(E2)*AJ1*VV1*U4/DSINH(E1)-DKK*(-BB)**2.*U3
     & *DCOSH(E2)*PAJ1*VV1*U4/DSINH(E1))*DEXP(DKK)

      AN2(II)=WET(II)*N*
     &((DKK*U3)**2*(CC**2.*DCOSH(E3)*PPAJ1*U4*VV2/DSINH(E1)
     &-(-BB)**2.*DCOSH(E2)*PPAJ1*VV1*U4/DSINH(E1))
     &+2*(PAJ1*DKK*U3*(DKK*CC**2.*U2*DSINH(E3)*U4*VV2
     &-DKK*(-BB)**2.*U2*DSINH(E2)*VV1*U4)/DSINH(E1))
     &+AJ1*(DKK*U2)**2*(CC**2.*DCOSH(E3)*VV2*U4/DSINH(E1)
     &-(-BB)**2.*DCOSH(E2)*VV1*U4/DSINH(E1)))*DEXP(DKK)

      AN3(II)=WET(II)*N*(-DKK*CC**2.*RAD(1)*U3*DSINH(E3)*AJ1*U4*VV2/
     &DSINH(E1)+DKK*CC**2.*RAD(1)*U2*DCOSH(E3)*PAJ1*VV2*U4/DSINH
     &(E1)+DKK*(-BB)**2.*RAD(1)*U3*DSINH(E2)*AJ1*VV1*U4/DSINH(E1)-
     &DKK*(-BB)**2.*RAD(1)*U2*DCOSH(E2)*PAJ1*VV1*U4/DSINH(E1))*
     & DEXP(DKK)

      AN4(II)=WET(II)*N*(-1*U5)*((CC)**2.*DCOSH(E3)*AJ1*VV2/DSINH(E1)-
     &(-BB)**2.*AJ1*VV1*DCOSH(E2)/DSINH(E1))*DEXP(DKK)

2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      SM4=0.D0

      DO 1999 IJ=1,IN
      SM1=SM1+AN1(IJ)
      SM2=SM2+AN2(IJ)
      SM3=SM3+AN3(IJ)
      SM4=SM4+AN4(IJ)
1999  CONTINUE
      RETURN
      END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                    FOR LINEAR CONCENTRATION PROFILE                    C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


      SUBROUTINE XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3,SM4)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN4(96),RAD(2),AN1(96),AN2(96),AN3(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      E2=DDK(II)*(ZZ-CC)
      E1=DDK(II)*(BB+CC)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      DK2=DKK*RAD(1)*U2
      CALL BESSEL(DK,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      PAJ0=-AJ1
      AJ3=4*AJ2/DK-AJ1
      PPAJ1=(-3*AJ1/4+AJ3/4)
      CALL BEST(N,1,1,0,DKK,-BB,VV1)
      CALL BEST (N,1,1,0,DKK,CC,VV2)
      AN1(II)=WET(II)*(-DKK)*(DKK*CC**2.*U2*DCOSH(E3)*AJ1*U4*VV2/DSINH(
     & E1)+DKK*CC**2.*U3*DSINH(E3)*PAJ1*VV2*U4/DSINH(E1)-DKK*
     & (-BB)**2.*U2*DCOSH(E2)*AJ1*VV1*U4/DSINH(E1)-DKK*(-BB)**2.*U3
     & *DSINH(E2)*PAJ1*VV1*U4/DSINH(E1))*DEXP(DKK)
      AN2(II)=WET(II)*(-DKK)*
     &((DKK*U3)**2*(CC**2.*DSINH(E3)*PPAJ1*U4*VV2/DSINH(E1)
     &-(-BB)**2.*DSINH(E2)*PPAJ1*VV1*U4/DSINH(E1))
     &+2*(PAJ1*DKK*U3*(DKK*CC**2.*U2*DCOSH(E3)*U4*VV2
     &-DKK*(-BB)**2.*U2*DCOSH(E2)*VV1*U4)/DSINH(E1))
     &+AJ1*(DKK*U2)**2*(CC**2.*DSINH(E3)*VV2*U4/DSINH(E1)
     &-(-BB)**2.*DSINH(E2)*VV1*U4/DSINH(E1)))*DEXP(DKK)

      AN3(II)=WET(II)*(-DKK)*(-DKK*CC**2.*RAD(1)*U3*DCOSH(E3)*AJ1
     &*U4*VV2/DSINH(E1)+DKK*CC**2.*RAD(1)*U2*DSINH(E3)*PAJ1*VV2*U4
     &/DSINH(E1)+DKK*(-BB)**2.*RAD(1)*U3*DCOSH(E2)*AJ1*VV1*U4/DSINH(E1)-
     &DKK*(-BB)**2.*RAD(1)*U2*DSINH(E2)*PAJ1*VV1*U4/DSINH(E1))*
     & DEXP(DKK)

      AN4(II)=WET(II)*(-DKK)*(-1*U5)*((CC)**2.*DSINH(E3)*AJ1*VV2
     &/DSINH(E1)-(-BB)**2.*AJ1*VV1*DSINH(E2)/DSINH(E1))*DEXP(DKK)

2001  CONTINUE
```

```
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      SM4=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN1(IJ)
      SM2=SM2+AN2(IJ)
      SM3=SM3+AN3(IJ)
      SM4=SM4+AN4(IJ)
1999  CONTINUE
      RETURN
      END
```

Appendix E2-1: Computer programming source code for estimating the osmo-phoretic velocity of single spherical particle parallel one solute impenetrable plate.

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION BF(900,3),WET(96)
      DIMENSION RAD(2),A(500,501),DDK(96),B(500,501)
      INTEGER GGG,T,GG,NX,LL1,LL2,LBB,LCC
      OPEN (23,FILE='GAUSS80.DAT',STATUS='OLD')
      OPEN (25,FILE='DTTH-0-0.TXT',STATUS='NEW')
      OPEN (24,FILE='WET3.DAT',STATUS='OLD')
      IN=80
      BB=0.1D0
      DO 1001 I=1,IN
      READ (23,*) DDK(I),WET(I)
1001  CONTINUE
      T=1
      PI=DACOS(-1.D0)
      FI=.01*PI/180.
      U4=DCOS(FI)
      U5=DSIN(FI)
      DO 3231 IUY=1,50
      READ(24,*) CV,NX
      RAD(1)=CV*BB
      R2=RAD(1)
      KAPPA1=0.D0
      KAPPA2=0.D0

      GGG=2*NX
      DO 511 I=1,T
      DO 512 J=1,NX
      NU=J+NX*(I-1)
      NY=J+NX*(I-1)+T*NX
      DO 513 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      B(NU,GGG+1)=U3*U4
      B(NY,GGG+1)=U3*U4

      DO 514 N=1,NX
      NZ=(2*N-1)+2*NX*(K-1)
      NL=2*N+2*NX*(K-1)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1)
      CALL XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM0,SM1,SM2
     &,SM3,SM4)

      B(NU,NZ)=(KAPPA2/R2)*(R2**(-N-1)*W1*U4+SM0)
      B(NU,NL)=-1.*(KAPPA2/R2)*(R2**N*W1*U4)-N*R2**(N-1)*W1*U4
      B(NY,NZ)=(KAPPA1/R2)*(R2**(-N-1)*W1*U4+SM0)
     & -((-N-1)*R2**(-N-2)*W1*U4+SM1)
      B(NY,NL)=-1.*(KAPPA1/R2)*(R2**(N)*W1*U4)

514   CONTINUE
513   CONTINUE
512   CONTINUE
511   CONTINUE
```

```
      LL1=500
      LL2=501
      LBB=GGG
      LCC=GGG+1
      CALL GAUSL(LL1,LL2,LBB,LCC,B)

      GG=T*NX
      DO 7765 NN=1,3
      DO 111 I=1,T
      DO 112 J=1,NX
      NO=J+NX*(I-1)
      NP=J+NX*(I-1)+T*NX
      NQ=J+NX*(I-1)+2*T*NX

      DO 113 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)

      IF(NN.EQ.1) THEN
      A(NO,3*GG+1)=1.D0
      A(NP,3*GG+1)=0.D0
      A(NQ,3*GG+1)=0.D0
      END IF

      IF(NN .EQ. 2) THEN
      A(NO,3*GG+1)=U2
      A(NP,3*GG+1)=0.D0
      A(NQ,3*GG+1)=-1*U3*U4
      END IF

      DO 114 N=1,NX
      NE=(3*N-2)+3*NX*(K-1)
      NF=(3*N-1)+3*NX*(K-1)
      NG=(3*N-0)+3*NX*(K-1)
      CALL FUCK1(U2,N,W,WW,WWW)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1)
      CALL FUCK3(U2,N,W2,WW2,WWW2)
      CALL XXD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SUM1,SUM2,SUM3,SUM4,
     & SUM5,SUM6,SUM7,SUM8,SUM9)
      A(NO,NE)=((2.*N*(2*N-1)*U3*W1*U4**2.+(N-2)*WW2*DCOS(2.*FI)-N*(N+1)
     & *(N-2)*WW)/2./R2**(N))+SUM1
      A(NO,NF)=(-1.*(WWW2*DCOS(2.*FI)-N*(N+1)*WWW)/2./R2**(N+2)+SUM2)
      A(NO,NG)=((W2*DCOS(2.*FI)+N*(N+1)*W)/2./R2**(N+1)+SUM3)
      A(NP,NE)=(N*(2*N-1)*U3*W1+(N-2)*WW2)*U4*U5/R2**(N)+SUM4
      A(NP,NF)=-(WWW2*U4*U5)/R2**(N+2)+SUM5
      A(NP,NG)=(W2*U4*U5)/R2**(N+1)+SUM6
      A(NQ,NE)=((N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U4/R2**N+SUM7)
      A(NQ,NF)=(-(N*WWW1*U4)/R2**(N+2)+SUM8)
      A(NQ,NG)=(-(W1*U4)/R2**(N+1)+SUM9)

114   CONTINUE
113   CONTINUE
112   CONTINUE
111   CONTINUE

      IF(NN.EQ.3)THEN
      DO 811 J=1,NX
      NO=J
```

```
      NP=J+NX
      NQ=J+2*NX
      CALL FU(1,J,1,NX,RAD,PI,U2,U3,R2)
      VALUE=0.D0
      VALUE1=0.D0
      DO 713 KK=1,NX
      NZ=2*KK-1
      NL=2*KK

      CALL FUCK2(U2,KK,W1,WW1,WWW1,PW1)
      CALL XRD(KK,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM0,SM1,SM2
     &,SM3,SM4)
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      VALUE=VALUE+B(NZ,GGG+1)*(R2**(-1*(KK+1))*W1*U4+SM0)
      VALUE1=VALUE1+B(NL,GGG+1)*(R2**(KK)*W1*U4)

713   CONTINUE
      A(NO,3*GG+1)=(VALUE-VALUE1)*U3*U4
      A(NP,3*GG+1)=(VALUE-VALUE1)*U3*U5
      A(NQ,3*GG+1)=(VALUE-VALUE1)*U2

811   CONTINUE
      END IF
      LL1=500
      LL2=501
      LBB=3*GG
      LCC=3*GG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,A)
      DO 999 I=1,3*GG
      BF(I,NN)=A(I,3*GG+1)
999   CONTINUE
7765  CONTINUE
      VVU=-R2/(2.D0+2.D0*KAPPA2+1.D0*KAPPA1)
      XN=NX
      HGD=-1*(BF(1,3)*BF(3,2)-BF(1,2)*BF(3,3))/
      &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      HGR=-1*(BF(1,1)*BF(3,3)-BF(1,3)*BF(3,1))/
      &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      WRITE (*,9)CV,HGD,HGR,XN
      WRITE (25,9)CV,HGD,HGR,XN
3231  CONTINUE
9     FORMAT (4(F12.6))
      STOP
      END

      SUBROUTINE FU(I,J,K,X,RAD,PI,U2,U3,R2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION RAD(2)
      INTEGER X
      PID=1.D-3
      DTHETA=(PI-4.D0*PID)/(X-2)
      IF(J==1) THEN
      Z=RAD(I)*DCOS(PID)
      V=RAD(I)*DSIN(PID)
      END IF
      IF((1<J) .AND. (J<=X/2)) THEN
```

```
      Z=RAD(I)*DCOS(PID+(J-1)*DTHETA)
      V=RAD(I)*DSIN(PID+(J-1)*DTHETA)
      END IF
      IF(X/2<J) THEN
      Z=RAD(I)*DCOS(PI/2.D0+(J-1-X/2)*DTHETA)
      V=RAD(I)*DSIN(PI/2.D0+(J-1-X/2)*DTHETA)
      END IF
      U2=Z/RAD(I)
      U3=V/RAD(I)
      R2=RAD(I)
      RETURN
      END

      SUBROUTINE GAUSL (N,M,II,JJ,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(N,M)
      DO 10 I=1,II
      AA=0.E0
      DO 9 J=1,II
    9 AA=AA+ABS(A(I,J))
      DO 10 J=1,JJ
   10 A(I,J)=A(I,J)/AA
      CALL XXXXX (N,M,II,JJ-II,A)
      RETURN
      END

      SUBROUTINE XXXXX (ND,NCOL,N,NS,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(ND,NCOL)
      N1=N+1
      NT=N+NS
      IF(N.EQ.1) GO TO 50
      DO 10 I=2,N
      IP=I-1
      I1=IP
      X=ABS(A(I1,I1))
      DO 11 J=I,N
      IF(ABS(A(J,I1)).LT.X) GO TO 11
      X=ABS(A(J,I1))
      IP=J
   11 CONTINUE
      IF(IP.EQ.I1) GO TO 13
      DO 12 J=I1,NT
      X=A(I1,J)
      A(I1,J)=A(IP,J)
   12 A(IP,J)=X
   13 DO 10 J=I,N
      X=A(J,I1)/A(I1,I1)
      DO 10 K=I,NT
   10 A(J,K)=A(J,K)-X*A(I1,K)
   50 DO 20 IP=1,N
      I=N1-IP
      DO 20 K=N1,NT
      A(I,K)=A(I,K)/A(I,I)
      IF(I.EQ.1) GO TO 20
      I1=I-1
      DO 25 J=1,I1
   25 A(J,K)=A(J,K)-A(I,K)*A(J,I)
```

```
   20 CONTINUE
      RETURN
      END

      SUBROUTINE FUCK2(U2,N,W1,WW1,WWW1,PW1)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PA(0:600)
      PA(0)=0.D0
      PA(1)=(1.-U2**2)**.5
      PA(2)=3.*U2*(1.-U2**2)**.5
      DO 100 J=1,N+1
      PA(J+1)=((2*J+1)*U2*PA(J)-(J+1)*PA(J-1))/(J)
100   CONTINUE
      W1=PA(N)
      WW1=PA(N-1)
      WWW1=PA(N+1)
      PW1=(N*U2*PA(N)-(N+1)*PA(N-1))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK1(U2,N,W,WW,WWW)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PR(0:550)
      PR(0)=1.D0
      PR(1)=U2
      DO 34 I=2,N+1
      PR(I)=((2*I-1)*U2*PR(I-1)-(I-1)*PR(I-2))/I
34    CONTINUE
      W=PR(N)
      WW=PR(N-1)
      WWW=PR(N+1)
      RETURN
      END

      SUBROUTINE FUCK3(U2,N,W2,WW2,WWW2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PA(0:600)
      PA(0)=0.D0
      PA(1)=0.D0
      PA(2)=3.*(1.-U2**2)
      DO 150 K=2,N+1
      PA(K+1)=((2*K+1)*U2*PA(K)-(K+2)*PA(K-1))/(K-1)
150   CONTINUE
      W2=PA(N)
      WW2=PA(N-1)
      WWW2=PA(N+1)
      RETURN
      END

      SUBROUTINE XXD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SUM1,SUM2,SUM3
     & ,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AAN(96),RAD(2)
      DIMENSION AAN1(96),AAN6(96),AAN7(96)
      DIMENSION AAN2(96),AAN5(96),AAN8(96)
      DIMENSION AAN3(96),AAN4(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
```

```
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      B1=AJ0*XX**2.+(YY**2.-XX**2.)*AJ1/DK
      B2=(AJ0-2.*AJ1/DK)/DK**2.
      G5E=DEXP(-1.*E3)
      G6DE=-1.*E3*DEXP(-1.*E3)
      G1DE=-1.*E3*DEXP(-1.*E3)
      G2DE=E3*DEXP(-1.*E3)
      G3DE=(1.-E3)*DEXP(-1.*E3)
      G4DE=(1.+E3)*DEXP(-1.*E3)
      CALL BEST(N,1,1,0,DKK,-BB,V1)
      CALL BEST(N,1,2,1,DKK,-BB,V2)
      CALL BEST(N-1,2,2,3,DKK,-BB,V3)
      CALL BEST(N-1,0,0,1,DKK,-BB,V4)
      CALL BEST(N-1,2,2,1,DKK,-BB,V9)
      CALL BEST(N-1,1,1,0,DKK,-BB,V11)
      H1B=-N*(2*N-1)*((-BB)**2.)*AJ0*V1+N*(2*N-1)*((-BB)**2.)*B1*V2/
     *DK1**2.-.5*(N-2)*(YY**2.-XX**2.)*B2*V3+.5*N*(N+1)*(N-2)*AJ0*V4
      H2B=(-N*(2*N-1)*((-BB)**2.)*(V1-V2)+.5*(N-2)*((-BB)**2.)
     * *V9+.5*N*(N+1)*(N-2)*V4)*B1/DK1**2.
      H3B=(DKK*(-BB)**2.)*(-N*(2*N-1)*(-BB)*V1+(N+1)*(N-2)*V11)*B1/
     & DK1**2.
      AAN(II)=WET(II)*(G5E*H1B+G6DE*H2B+G1DE*H3B)*DEXP(DDK(II))
      CALL BEST(N+1,2,2,3,DKK,-BB,S1)
      CALL BEST(N+1,0,0,1,DKK,-BB,S2)
      CALL BEST(N+1,2,2,1,DKK,-BB,S5)
      CALL BEST(N+1,0,0,1,DKK,-BB,S6)
      CALL BEST(N+1,1,1,0,DKK,-BB,S9)
      H4B=.5*((YY**2.-XX**2.)*B2*S1-N*(N+1)*AJ0*S2)
      H5B=-.5*(((-BB)**2.)*S5+N*(N+1)*S6)*B1/DK1**2.
      H6B=N*DKK*((-BB)**2.)*B1*S9/DK1**2.
      AAN1(II)=WET(II)*(G5E*H4B+G6DE*H5B+G1DE*H6B)*DEXP(DDK(II))
      CALL BEST(N,2,2,3,DKK,-BB,F1)
      CALL BEST(N,0,0,1,DKK,-BB,F2)
      CALL BEST(N,2,2,1,DKK,-BB,F5)
      CALL BEST(N,0,0,1,DKK,-BB,F6)
      CALL BEST(N,1,1,0,DKK,-BB,F9)
      H7B=-.5*((YY**2.-XX**2.)*B2*F1+N*(N+1)*AJ0*F2)
      H8B=.5*(((-BB)**2.)*F5-N*(N+1)*F6)*B1/DK1**2.
      H9B=DKK*((-BB)**2.)*B1*F9/DK1**2.
      AAN2(II)=WET(II)*(G5E*H7B+G6DE*H8B+G1DE*H9B)*DEXP(DDK(II))
      CALL BEST(N,1,1,2,DKK,-BB,Z1)
      CALL BEST(N-1,2,2,3,DKK,-BB,Z2)
      CALL BEST(N-1,0,0,3,DKK,-BB,Z3)
      CALL BEST(N,1,2,3,DKK,-BB,Z7)
      CALL BEST(N-1,1,1,2,DKK,-BB,Z9)
      H10B=XX*YY*B2*(-N*(2*N-1)*Z1-.5*(N-2)*Z2+N*(N+1)*(N-2)*Z3/2./
     * (-BB)**2.)
      H11B=XX*YY*B2*(N*(2*N-1)*Z7+(N-2)*Z2)
      H12B=DKK*XX*YY*B2*(-N*(2*N-1)*(-BB)*Z1+(N+1)*(N-2)*Z9)
      AAN3(II)=WET(II)*(G6DE*H10B+G3DE*H11B+G1DE*H12B)*DEXP(DDK(II))
      CALL BEST(N+1,2,2,3,DKK,-BB,C1)
      CALL BEST(N+1,0,0,3,DKK,-BB,C2)
```

```
      CALL BEST(N+1,1,1,2,DKK,-BB,C3)
      H13B=.5*XX*YY*B2*(C1-N*(N+1)*C2/(-BB)**2.)
      H14B=-1.*XX*YY*B2*C1
      H15B=N*DKK*XX*YY*B2*C3
      AAN4(II)=WET(II)*(G6DE*H13B+G3DE*H14B+G1DE*H15B)*DEXP(DDK(II))
      CALL BEST(N,2,2,3,DKK,-BB,Q1)
      CALL BEST(N,0,0,3,DKK,-BB,Q2)
      CALL BEST(N,1,1,2,DKK,-BB,Q3)
      H16B=-.5*XX*YY*B2*(Q1+N*(N+1)*Q2/(-BB)**2.)
      H17B=XX*YY*B2*Q1
      H18B=DKK*XX*YY*B2*Q3
      AAN5(II)=WET(II)*(G6DE*H16B+G3DE*H17B+G1DE*H18B)*DEXP(DDK(II))
      CALL BEST(N,1,1,2,DKK,-BB,Y1)
      CALL BEST(N,1,2,3,DKK,-BB,Y2)
      CALL BEST(N-1,2,2,3,DKK,-BB,Y3)
      CALL BEST(N-1,0,0,3,DKK,-BB,Y4)
      CALL BEST(N-1,1,1,2,DKK,-BB,Y9)
      H19B=-1.*XX*AJ1*(N*(2*N-1)*(Y1-Y2)-.5*(N-2)*Y3-.5*N*(N+1)*(N-2)*
     * Y4/(-BB)**2.)/DKK**2./DK1
      H20B=-1.*XX*AJ1*(N*(2*N-1)*(-BB)*Y1-(N+1)*(N-2)*Y9)/DK1/DKK
      AAN6(II)=WET(II)*(G2DE*H19B+G4DE*H20B)*DEXP(DDK(II))
      CALL BEST(N+1,2,2,3,DKK,-BB,UU1)
      CALL BEST(N+1,0,0,3,DKK,-BB,UU2)
      CALL BEST(N+1,1,1,2,DKK,-BB,UU3)
      H21B=-.5*XX*AJ1*(UU1+N*(N+1)*UU2/(-BB)**2.)/DKK**2./DK1
      H22B=N*XX*AJ1*UU3/DK1/DKK
      AAN7(II)=WET(II)*(G2DE*H21B+G4DE*H22B)*DEXP(DDK(II))
      CALL BEST(N,2,2,3,DKK,-BB,AW1)
      CALL BEST(N,0,0,3,DKK,-BB,AW2)
      CALL BEST(N,1,1,2,DKK,-BB,AW3)
      H23B=.5*XX*AJ1*(AW1-N*(N+1)*AW2/(-BB)**2.)/DKK**2./DK1
      H24B=XX*AJ1*AW3/DK1/DKK
      AAN8(II)=WET(II)*(G2DE*H23B+G4DE*H24B)*DEXP(DDK(II))
2001  CONTINUE
      SUM1=0.D0
      SUM2=0.D0
      SUM3=0.D0
      SUM4=0.D0
      SUM5=0.D0
      SUM6=0.D0
      SUM7=0.D0
      SUM8=0.D0
      SUM9=0.D0
      DO 1999 IJ=1,IN
      SUM1=SUM1+AAN(IJ)
      SUM2=SUM2+AAN1(IJ)
      SUM3=SUM3+AAN2(IJ)
      SUM4=SUM4+AAN3(IJ)
      SUM5=SUM5+AAN4(IJ)
      SUM6=SUM6+AAN5(IJ)
      SUM7=SUM7+AAN6(IJ)
      SUM8=SUM8+AAN7(IJ)
      SUM9=SUM9+AAN8(IJ)
1999  CONTINUE
      RETURN
      END

      SUBROUTINE BEST(N,M,J,L,ABK,ZZ1,BBB)
```

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PI=DACOS(-1.D0)
      FFD=0.D0
      DO 104 IQ=0,N/2
      CALL GAMMA(N-2*IQ-M,AA1)
      CALL GAMMA(IQ,AA2)
      XZ=ABK*ABS(ZZ1)
      CALL AKV(N,IQ,J,XZ,WK)
      FFD1=((2/PI)**.5)/((-2.D0)**IQ)/AA2/AA1/(ZZ1)**(N+M)
      IF (N-2*IQ-M .LT. 0) THEN
      FFD1=0.D0
      END IF
      FFD=FFD+FFD1*WK*(ABK*ABS(ZZ1))**(N-IQ+L-.5)
104   CONTINUE
      BBB=FFD
      IF (N .LT. M) THEN
      BBB=0.D0
      END IF
      RETURN
      END

      SUBROUTINE AKV(N,IQ,J,X,FDK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION AAK(-20:80),FFK(-20:80)
      IF (N-IQ-J .GE. 1) THEN
      NN=N-IQ-J-1
      ELSE
      NN=N-IQ-J
      END IF
      PI=DACOS(-1.D0)
      AAK(0)=-1.*(.5D0*PI/X)/DEXP(X)
      AAK(1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      AAK(-1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(-2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(0)=(.5D0*PI/X)**.5/DEXP(X)
      FFK(1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(-1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(-2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      IF (IABS(NN) .LE. 2 ) THEN
      GO TO 2233
      END IF
      DO 502 I=3,IABS(NN)
      AAK(I)=AAK(I-2)-(2*I-1)*AAK(I-1)/X
      FFK(I)=AAK(I)/(-1.)**(I+1)/(.5*PI/X)**.5
      FFK(-I)=FFK(I)
502   CONTINUE
2233  CONTINUE
      FDK=FFK(NN)
4443  CONTINUE
      RETURN
      END

      SUBROUTINE GAMMA(J,AJK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IF (J .LE. 0) THEN
      AJK=1.D0
```

```
        ELSE
        AJK=1.D0
        DO 300 I=1,J
        SS=DBLE(I)
        AJK=AJK*SS
300   CONTINUE
      END IF
      RETURN
      END

      SUBROUTINE BESSEL(CX,AJ,AJ0,AJ1,AJ2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      AJ0=0.D0
      AJ1=0.D0
      AJ2=0.D0
      DO 100 J=0,80
      CALL GAMMA(J,AJK)
      TJ=AJ0
      AJ0=AJ0+((-1.D0)**J)*(CX/2.)**(2*J)/(AJK)**2.
      IF (ABS(AJ0-TJ) .LE. 0.000000000000001 ) THEN
      GO TO    500
      END IF
100   CONTINUE
500   CONTINUE
      DO 107 J=0,80
      CALL GAMMA(J,AJK)
      TJ1=AJ1
      AJ1=AJ1+((-1.D0)**J)*(CX/2.)**(2*J+1)/((AJK)**2.)/(J+1)
      IF (ABS(AJ1-TJ1) .LE. 0.000000000000001 ) THEN
      GO TO 201
      END IF
107   CONTINUE
201   CONTINUE
      DO 108 J=0,80
      CALL GAMMA(J,AJK)
      TJ2=AJ2
      AJ2=AJ2+((-1.D0)**J)*(CX/2.)**(2*J+2)/((AJK)**2.)/(J+1)
     &/(J+2)
      IF (ABS(AJ2-TJ2)    .LE. 0.0000000000000001) THEN
      GO TO 200
      END IF
108   CONTINUE
200   CONTINUE
        AJ=-1.*AJ1
        RETURN
        END

      SUBROUTINE XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM0,SM1,SM2
     &,SM3,SM4)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN4(96),RAD(2),AN1(96),AN2(96),AN3(96)
      DIMENSION AN0(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=-1.D0*DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
```

```
      DKK=DDK(II)
      DK1=RAD(1)*U3
      DK2=DKK*RAD(1)*U2
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      PAJ0=-AJ1
      AJ3=4*AJ2/DK-AJ1
      PPAJ1=(-3*AJ1/4+AJ3/4)
      CALL BEST(N+1,1,1,0,DKK,-BB,VV1)
      AN0(II)=WET(II)*N*(U4)*(
     &-1.D0*(-BB)**2.*AJ1*VV1*DEXP(E3))*DEXP(DKK)
      AN1(II)=WET(II)*N*(
     &DKK*(-BB)**2.*U2*DEXP(E3)*AJ1*VV1*U4-DKK*(-BB)**2.*U3
     &*DEXP(E3)*PAJ1*VV1*U4)*DEXP(DKK)
      AN2(II)=WET(II)*N*
     &((DKK*U3)**2.*(
     &-(-BB)**2.*DEXP(E3)*PPAJ1*VV1*U4)
     &+2*(PAJ1*DKK*U3*(
     &+DKK*(-BB)**2.*U2*DEXP(E3)*VV1*U4))
     &+AJ1*(DKK*U2)**2*(
     &-(-BB)**2.*DEXP(E3)*VV1*U4))*DEXP(DKK)
      AN3(II)=WET(II)*N*(
     &-DKK*(-BB)**2.*RAD(1)*U3*DEXP(E3)*AJ1*VV1*U4-
     &DKK*(-BB)**2.*RAD(1)*U2*DEXP(E3)*PAJ1*VV1*U4)*
     &DEXP(DKK)
      AN4(II)=WET(II)*N*(-1*U5)*(
     &-1.D0*(-BB)**2.*AJ1*VV1*DEXP(E3))*DEXP(DKK)

2001  CONTINUE
      SM0=0.D0
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      SM4=0.D0

      DO 1999 IJ=1,IN
      SM0=SM0+AN0(IJ)
      SM1=SM1+AN1(IJ)
      SM2=SM2+AN2(IJ)
      SM3=SM3+AN3(IJ)
      SM4=SM4+AN4(IJ)
1999  CONTINUE
      RETURN
      END




CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                 FOR LINEAR CONCENTRATION PROFILE                  C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

      SUBROUTINE XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM0,SM1,SM2
     &,SM3,SM4)
```

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN4(96),RAD(2),AN1(96),AN2(96),AN3(96)
      DIMENSION AN0(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=-1.D0*DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      DK2=DKK*RAD(1)*U2
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      PAJ0=-AJ1
      AJ3=4*AJ2/DK-AJ1
      PPAJ1=(-3*AJ1/4+AJ3/4)
      CALL BEST(N,1,1,0,DKK,-BB,VV1)
      AN0(II)=WET(II)*(-DKK)*(U4)*(
     &(-BB)**2.*AJ1*VV1*DEXP(E3))*DEXP(DKK)

      AN1(II)=WET(II)*(-DKK)*(
     &-DKK*(-BB)**2.*U2*DEXP(E3)*AJ1*VV1*U4+DKK*(-BB)**2.*U3
     &*DEXP(E3)*PAJ1*VV1*U4)*DEXP(DKK)
      AN2(II)=WET(II)*(-DKK)*
     &((DKK*U3)**2.*
     &(-BB)**2.*DEXP(E3)*PPAJ1*VV1*U4
     &-2*PAJ1*DKK*U3*DKK*(-BB)**2.*U2*DEXP(E3)*VV1*U4
     &+AJ1*(DKK*U2)**2*(-BB)**2.*DEXP(E3)*VV1*U4)*DEXP(DKK)
      AN3(II)=WET(II)*(-DKK)*(
     &DKK*(-BB)**2.*RAD(1)*U3*DEXP(E3)*AJ1*VV1*U4+
     &DKK*(-BB)**2.*RAD(1)*U2*DEXP(E3)*PAJ1*VV1*U4)*
     &DEXP(DKK)
      AN4(II)=WET(II)*(-DKK)*(-1*U5)*(
     &(-BB)**2.*AJ1*VV1*DEXP(E3))*DEXP(DKK)

2001  CONTINUE
      SM0=0.D0
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      SM4=0.D0

      DO 1999 IJ=1,IN
      SM0=SM0+AN0(IJ)
      SM1=SM1+AN1(IJ)
      SM2=SM2+AN2(IJ)
      SM3=SM3+AN3(IJ)
      SM4=SM4+AN4(IJ)
1999  CONTINUE
      RETURN
      END
```

Appendix E2-2: Computer programming source code for estimating the osmo-phoretic velocity of one spherical particle parallel two solute impenetrable plates.

```
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(500,501),RAD(2),DDK(96),WET(96),B(500,501), BF(500,3)
      INTEGER GGG,T,GG,NX,LL1,LL2,LBB,LCC
      OPEN (23,FILE='GAUSS80.DAT',STATUS='OLD')
      OPEN (25,FILE='DDTTH-0-10.TXT',STATUS='NEW')
      OPEN (24,FILE='WET3.DAT',STATUS='OLD')
      IN=80
      BB=0.1D0
      TR=1.D0
      CC=BB*TR
      DO 1001 I=1,IN
      READ (23,*) DDK(I),WET(I)
1001  CONTINUE
      T=1
      PI=DACOS(-1.D0)
      FI=.01*PI/180.
      U4=DCOS(FI)
      U5=DSIN(FI)
      DO 3231 IUY=1,50
      READ (24,*) CV,NX
      RAD(1)=CV*BB
      R2=RAD(1)
      KAPPA1=0.D0
      KAPPA2=10.D0
      GGG=2*NX
      DO 511 I=1,T
      DO 512 J=1,NX
      NU=J+NX*(I-1)
      NY=J+NX*(I-1)+T*NX
      DO 513 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      B(NU,GGG+1)=U3*U4
      B(NY,GGG+1)=U3*U4
      DO 514 N=1,NX
      NZ=(2*N-1)+2*NX*(K-1)
      NL=2*N+2*NX*(K-1)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM0,SM1,
     &SM2,SM3,SM4)
      B(NU,NZ)=(KAPPA2/R2)*(R2**(-N-1)*W1*U4+SM0)
      B(NU,NL)=-1.*(KAPPA2/R2)*(R2**N*W1*U4)-N*R2**(N-1)*W1*U4
      B(NY,NZ)=(KAPPA1/R2)*(R2**(-N-1)*W1*U4+SM0)
     &-((-N-1)*R2**(-N-2)*W1*U4+SM1)
      B(NY,NL)=-1.*(KAPPA1/R2)*(R2**(N)*W1*U4)
514   CONTINUE
513   CONTINUE
512   CONTINUE
511   CONTINUE
      LL1=500
      LL2=501
```

```
      LBB=GGG
      LCC=GGG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,B)
      GG=T*NX
      DO 7765 NN=1,3
      DO 111 I=1,T
      DO 112 J=1,NX
      NO=J+NX*(I-1)
      NP=J+NX*(I-1)+T*NX
      NQ=J+NX*(I-1)+2*T*NX
      DO 113 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)

      IF(NN .EQ. 1) THEN
      A(NO,3*GG+1)=1.D0
      A(NP,3*GG+1)=0.D0
      A(NQ,3*GG+1)=0.D0
      END IF

      IF(NN .EQ. 2) THEN
      A(NO,3*GG+1)=U2
      A(NP,3*GG+1)=0.D0
      A(NQ,3*GG+1)=-1*U3*U4
      END IF

      DO 114 N=1,NX
      NE=(3*N-2)+3*NX*(K-1)
      NF=(3*N-1)+3*NX*(K-1)
      NG=(3*N-0)+3*NX*(K-1)
      CALL FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
      CALL XXD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,
     &SUM1,SUM2,SUM3,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9)
      A(NO,NE)=((2.*N*(2*N-1)*U3*W1*U4**2.+(N-2)*WW2*DCOS(2.*FI)-
     &N*(N+1)*(N-2)*WW)/2./R2**(N))+SUM1
      A(NO,NF)=(-1.*(WWW2*DCOS(2.*FI)-
     &N*(N+1)*WWW)/2./R2**(N+2)+SUM2)
      A(NO,NG)=((W2*DCOS(2.*FI)+N*(N+1)*W)/2./R2**(N+1)+SUM3)
      A(NP,NE)=(N*(2*N-1)*U3*W1+(N-2)*WW2)*U4*U5/R2**(N)+SUM4
      A(NP,NF)=-(WWW2*U4*U5)/R2**(N+2)+SUM5
      A(NP,NG)=(W2*U4*U5)/R2**(N+1)+SUM6
      A(NQ,NE)=((N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U4/R2**N+SUM7)
      A(NQ,NF)=(-(N*WWW1*U4)/R2**(N+2)+SUM8)
      A(NQ,NG)=(-(W1*U4)/R2**(N+1)+SUM9)
114   CONTINUE
113   CONTINUE
112   CONTINUE
111   CONTINUE

      IF(NN .EQ. 3) THEN
      DO 811 J=1,NX
      NO=J
      NP=J+NX
      NQ=J+2*NX
      CALL FU(1,J,1,NX,RAD,PI,U2,U3,R2)
      VALUE=0.D0
      VALUE1=0.D0
```

```
      DO 713 KK=1,NX
      NZ=2*KK-1
      NL=2*KK
      CALL FUCK2(U2,KK,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL XRD(KK,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM0,SM1,
     &SM2,SM3,SM4)
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      VALUE=VALUE+B(NZ,GGG+1)*(R2**(-1*(KK+1))*W1*U4+SM0)
      VALUE1=VALUE1+B(NL,GGG+1)*(R2**(KK)*W1*U4)
713   CONTINUE
      A(NO,3*GG+1)=(VALUE-VALUE1)*U3*U4
      A(NP,3*GG+1)=(VALUE-VALUE1)*U3*U5
      A(NQ,3*GG+1)=(VALUE-VALUE1)*U2
811   CONTINUE
      END IF
      LL1=500
      LL2=501
      LBB=3*GG
      LCC=3*GG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,A)
      DO 999 I=1,3*GG
      BF(I,NN)=A(I,3*GG+1)
999   CONTINUE
7765  CONTINUE
      VVU=-R2/(2.D0+2.D0*KAPPA2+1.D0*KAPPA1)
      WRITE(*,*) VVU
      XN=NX
      HGD=-1*(BF(1,3)*BF(3,2)-BF(1,2)*BF(3,3))/
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      HGR=-1*(BF(1,1)*BF(3,3)-BF(1,3)*BF(3,1))/
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      WRITE (*,9)CV,HGD,HGR,XN
      WRITE (25,9)CV,HGD,HGR,XN
3231  CONTINUE
9     FORMAT (5(F12.5))
      STOP
      END

      SUBROUTINE XXD(N,BB,CC,IN,RAD,U2,U3,U4, U5,DDK,WET,SUM1,
     &SUM2,SUM3,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AAN(96),RAD(2)
      DIMENSION AAN1(96),AAN6(96),AAN7(96)
      DIMENSION AAN2(96),AAN5(96),AAN8(96)
      DIMENSION AAN3(96),AAN4(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E1=DDK(II)*(BB+CC)
      E2=DDK(II)*(ZZ-CC)
      E3=DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ0,AJ1,AJ2)
```

```
  B1=AJ0*XX**2.+(YY**2.-XX**2.)*AJ1/DK
  B2=(AJ0-2.*AJ1/DK)/DK**2.
  DETA1=2.D0*DSINH(E1)
  DETA2=4.D0*((DSINH(E1))**2.-E1**2.)
  G5E=(-2.*DSINH(E2))/DETA1
  G5D=(-2.*DSINH(E3))/DETA1
  G6DE=8.*E1**2.*(E3*(DSINH(E1)/E1)*(DSINH(E3)/E3-DSINH(E1)*DCOSH
&(E2)/E1)+E2*(DSINH(E1)*DCOSH(E3)/E1-DSINH(E2)/E2))/DETA1/DETA2
  G6ED=8.*E1**2.*(E2*(DSINH(E1)/E1)*(DSINH(E2)/E2-DSINH(E1)*DCOSH
&(E3)/E1)+E3*(DSINH(E1)*DCOSH(E2)/E1-DSINH(E3)/E3))/DETA1/DETA2
  G1DE=4.*E1*E3*E2*(DSINH(E3)/E3
&+DSINH(E1)*DSINH(E2)/E1/E2)/DETA2
  G1ED=4.*E1*E2*E3*(DSINH(E2)/E2
&+DSINH(E1)*DSINH(E3)/E1/E3)/DETA2
  G2DE=4.*E1*E3*E2*(DSINH(E3)/E3-DSINH(E1)*DSINH(E2)/E1/E2)/DETA2
  G2ED=4.*E1*E2*E3*(DSINH(E2)/E2-DSINH(E1)*DSINH(E3)/E1/E3)/DETA2
  G3DE=4.*E1*(E2*(DCOSH(E3)-
&DSINH(E1)*DSINH(E2)/E1/E2)+E3*(SINH(E3)
&/E3-DSINH(E1)*DCOSH(E2)/E1))/DETA2
  G3ED=4.*E1*(E3*(DCOSH(E2)-
&DSINH(E1)*DSINH(E3)/E1/E3)+E2*(SINH(E2)
&/E2-DSINH(E1)*DCOSH(E3)/E1))/DETA2
  G4DE=4.*E1*(E2*(DCOSH(E3)-DSINH(E1)*DSINH(E2)/E1/E2)
&-E3*(SINH(E3)/E3-DSINH(E1)*DCOSH(E2)/E1))/DETA2
  G4ED=4.*E1*(E3*(DCOSH(E2)-DSINH(E1)*DSINH(E3)/E1/E3)
&-E2*(SINH(E2)/E2-DSINH(E1)*DCOSH(E3)/E1))/DETA2

  CALL BEST(N,1,1,0,DKK,-BB,V1)
  CALL BEST(N,1,2,1,DKK,-BB,V2)
  CALL BEST(N-1,2,2,3,DKK,-BB,V3)
  CALL BEST(N-1,0,0,1,DKK,-BB,V4)
  CALL BEST(N,1,1,0,DKK,CC,V5)
  CALL BEST(N,1,2,1,DKK,CC,V6)
  CALL BEST(N-1,2,2,3,DKK,CC,V7)
  CALL BEST(N-1,0,0,1,DKK,CC,V8)
  CALL BEST(N-1,2,2,1,DKK,-BB,V9)
  CALL BEST(N-1,2,2,1,DKK,CC,V10)
  CALL BEST(N-1,1,1,0,DKK,-BB,V11)
  CALL BEST(N-1,1,1,0,DKK,CC,V12)
  H1B=-N*(2*N-1)*((-BB)**2.)*AJ0*V1+N*(2*N-1)*((-BB)**2.)*B1*V2/
&DK1**2.-.5*(N-2)*(YY**2.-XX**2.)*B2*V3+.5*N*(N+1)*(N-2)*AJ0*V4
  H1C=-N*(2*N-1)*(CC**2.)*AJ0*V5+N*(2*N-1)*(CC**2.)*B1*V6/
&DK1**2.-.5*(N-2)*(YY**2.-XX**2.)*B2*V7+.5*N*(N+1)*(N-2)*AJ0*V8
  H2B=(-N*(2*N-1)*((-BB)**2.)*(V1-V2)+.5*(N-2)*((-BB)**2.)
&*V9+.5*N*(N+1)*(N-2)*V4)*B1/DK1**2.
  H2C=(-N*(2*N-1)*(CC**2.)*(V5-V6)+.5*(N-2)*(CC**2.)
&*V10+.5*N*(N+1)*(N-2)*V8)*B1/DK1**2.
  H3B=(DKK*(-BB)**2.)*(-N*(2*N-1)*(-BB)*V1+(N+1)*(N-2)*V11)*B1/
&DK1**2.
  H3C=(DKK*CC**2.)*(-N*(2*N-1)*CC*V5+(N+1)*(N-2)*V12)*B1/DK1**2.
  AAN(II)=WET(II)*(G5E*H1B-G5D*H1C+G6DE*H2B
&-G6ED*H2C+G1DE*H3B-G1ED*H3C)*DEXP(DDK(II))

  CALL BEST(N+1,2,2,3,DKK,-BB,S1)
  CALL BEST(N+1,0,0,1,DKK,-BB,S2)
  CALL BEST(N+1,2,2,3,DKK,CC,S3)
  CALL BEST(N+1,0,0,1,DKK,CC,S4)
  CALL BEST(N+1,2,2,1,DKK,-BB,S5)
```

```
  CALL BEST(N+1,0,0,1,DKK,-BB,S6)
  CALL BEST(N+1,2,2,1,DKK,CC,S7)
  CALL BEST(N+1,0,0,1,DKK,CC,S8)
  CALL BEST(N+1,1,1,0,DKK,-BB,S9)
  CALL BEST(N+1,1,1,0,DKK,CC,S10)
  H4B=.5*((YY**2.-XX**2.)*B2*S1-N*(N+1)*AJ0*S2)
  H4C=.5*((YY**2.-XX**2.)*B2*S3-N*(N+1)*AJ0*S4)
  H5B=-.5*(((-BB)**2.)*S5+N*(N+1)*S6)*B1/DK1**2.
  H5C=-.5*((CC**2.)*S7+N*(N+1)*S8)*B1/DK1**2.
  H6B=N*DKK*((-BB)**2.)*B1*S9/DK1**2.
  H6C=N*DKK*(CC**2.)*B1*S10/DK1**2.
  AAN1(II)=WET(II)*(G5E*H4B-G5D*H4C+G6DE*H5B
&-G6ED*H5C+G1DE*H6B-G1ED*H6C)*DEXP(DDK(II))

  CALL BEST(N,2,2,3,DKK,-BB,F1)
  CALL BEST(N,0,0,1,DKK,-BB,F2)
  CALL BEST(N,2,2,3,DKK,CC,F3)
  CALL BEST(N,0,0,1,DKK,CC,F4)
  CALL BEST(N,2,2,1,DKK,-BB,F5)
  CALL BEST(N,0,0,1,DKK,-BB,F6)
  CALL BEST(N,2,2,1,DKK,CC,F7)
  CALL BEST(N,0,0,1,DKK,CC,F8)
  CALL BEST(N,1,1,0,DKK,-BB,F9)
  CALL BEST(N,1,1,0,DKK,CC,F10)
  H7B=-.5*((YY**2.-XX**2.)*B2*F1+N*(N+1)*AJ0*F2)
  H7C=-.5*((YY**2.-XX**2.)*B2*F3+N*(N+1)*AJ0*F4)
  H8B=.5*(((-BB)**2.)*F5-N*(N+1)*F6)*B1/DK1**2.
  H8C=.5*((CC**2.)*F7-N*(N+1)*F8)*B1/DK1**2.
  H9B=DKK*((-BB)**2.)*B1*F9/DK1**2.
  H9C=DKK*(CC**2.)*B1*F10/DK1**2.
  AAN2(II)=WET(II)*(G5E*H7B-G5D*H7C+G6DE*H8B
&-G6ED*H8C+G1DE*H9B-G1ED*H9C)*DEXP(DDK(II))

  CALL BEST(N,1,1,2,DKK,-BB,Z1)
  CALL BEST(N-1,2,2,3,DKK,-BB,Z2)
  CALL BEST(N-1,0,0,3,DKK,-BB,Z3)
  CALL BEST(N,1,1,2,DKK,CC,Z4)
  CALL BEST(N-1,2,2,3,DKK,CC,Z5)
  CALL BEST(N-1,0,0,3,DKK,CC,Z6)
  CALL BEST(N,1,2,3,DKK,-BB,Z7)
  CALL BEST(N,1,2,3,DKK,CC,Z8)
  CALL BEST(N-1,1,1,2,DKK,-BB,Z9)
  CALL BEST(N-1,1,1,2,DKK,CC,Z10)
  H10B=XX*YY*B2*(-N*(2*N-1)*Z1-.5*(N-2)*Z2+N*(N+1)*(N-2)*Z3/2./
&(-BB)**2.)
  H10C=XX*YY*B2*(-N*(2*N-1)*Z4-.5*(N-2)*Z5+N*(N+1)*(N-2)*Z6/2/
&CC**2.)
  H11B=XX*YY*B2*(N*(2*N-1)*Z7+(N-2)*Z2)
  H11C=XX*YY*B2*(N*(2*N-1)*Z8+(N-2)*Z5)
  H12B=DKK*XX*YY*B2*(-N*(2*N-1)*(-BB)*Z1+(N+1)*(N-2)*Z9)
  H12C=DKK*XX*YY*B2*(-N*(2*N-1)*CC*Z4+(N+1)*(N-2)*Z10)
  AAN3(II)=WET(II)*(G6DE*H10B-G6ED*H10C+G3DE*H11B
&-G3ED*H11C+G1DE*H12B-G1ED*H12C)*DEXP(DDK(II))

  CALL BEST(N+1,2,2,3,DKK,-BB,C1)
  CALL BEST(N+1,0,0,3,DKK,-BB,C2)
  CALL BEST(N+1,1,1,2,DKK,-BB,C3)
  CALL BEST(N+1,2,2,3,DKK,CC,C4)
```

```
  CALL BEST(N+1,0,0,3,DKK,CC,C5)
  CALL BEST(N+1,1,1,2,DKK,CC,C6)
  H13B=.5*XX*YY*B2*(C1-N*(N+1)*C2/(-BB)**2.)
  H13C=.5*XX*YY*B2*(C4-N*(N+1)*C5/CC**2.)
  H14B=-1.*XX*YY*B2*C1
  H14C=-1.*XX*YY*B2*C4
  H15B=N*DKK*XX*YY*B2*C3
  H15C=N*DKK*XX*YY*B2*C6
  AAN4(II)=WET(II)*(G6DE*H13B-G6ED*H13C+G3DE*H14B
&-G3ED*H14C+G1DE*H15B-G1ED*H15C)*DEXP(DDK(II))

  CALL BEST(N,2,2,3,DKK,-BB,Q1)
  CALL BEST(N,0,0,3,DKK,-BB,Q2)
  CALL BEST(N,1,1,2,DKK,-BB,Q3)
  CALL BEST(N,2,2,3,DKK,CC,Q4)
  CALL BEST(N,0,0,3,DKK,CC,Q5)
  CALL BEST(N,1,1,2,DKK,CC,Q6)
  H16B=-.5*XX*YY*B2*(Q1+N*(N+1)*Q2/(-BB)**2.)
  H16C=-.5*XX*YY*B2*(Q4+N*(N+1)*Q5/CC**2.)
  H17B=XX*YY*B2*Q1
  H17C=XX*YY*B2*Q4
  H18B=DKK*XX*YY*B2*Q3
  H18C=DKK*XX*YY*B2*Q6
  AAN5(II)=WET(II)*(G6DE*H16B-G6ED*H16C+G3DE*H17B
&-G3ED*H17C+G1DE*H18B-G1ED*H18C)*DEXP(DDK(II))

  CALL BEST(N,1,1,2,DKK,-BB,Y1)
  CALL BEST(N,1,2,3,DKK,-BB,Y2)
  CALL BEST(N-1,2,2,3,DKK,-BB,Y3)
  CALL BEST(N-1,0,0,3,DKK,-BB,Y4)
  CALL BEST(N,1,1,2,DKK,CC,Y5)
  CALL BEST(N,1,2,3,DKK,CC,Y6)
  CALL BEST(N-1,2,2,3,DKK,CC,Y7)
  CALL BEST(N-1,0,0,3,DKK,CC,Y8)
  CALL BEST(N-1,1,1,2,DKK,-BB,Y9)
  CALL BEST(N-1,1,1,2,DKK,CC,Y10)
  H19B=-1.*XX*AJ1*(N*(2*N-1)*(Y1-Y2)-.5*(N-2)*Y3-.5*N*(N+1)*(N-2)*
&Y4/(-BB)**2.)/DKK**2./DK1
  H19C=-1.*XX*AJ1*(N*(2*N-1)*(Y5-Y6)-.5*(N-2)*Y7-.5*N*(N+1)*(N-2)*
&Y8/CC**2.)/DKK**2./DK1
  H20B=-1.*XX*AJ1*(N*(2*N-1)*(-BB)*Y1-(N+1)*(N-2)*Y9)/DK1/DKK
  H20C=-1.*XX*AJ1*(N*(2*N-1)*CC*Y5-(N+1)*(N-2)*Y10)/DK1/DKK
  AAN6(II)=WET(II)*(G2DE*H19B-G2ED*H19C+G4DE*H20B-G4ED*H20C)
&*DEXP(DDK(II))

  CALL BEST(N+1,2,2,3,DKK,-BB,UU1)
  CALL BEST(N+1,0,0,3,DKK,-BB,UU2)
  CALL BEST(N+1,1,1,2,DKK,-BB,UU3)
  CALL BEST(N+1,2,2,3,DKK,CC,UU4)
  CALL BEST(N+1,0,0,3,DKK,CC,UU5)
  CALL BEST(N+1,1,1,2,DKK,CC,UU6)
  H21B=-.5*XX*AJ1*(UU1+N*(N+1)*UU2/(-BB)**2.)/DKK**2./DK1
  H21C=-.5*XX*AJ1*(UU4+N*(N+1)*UU5/CC**2.)/DKK**2./DK1
  H22B=N*XX*AJ1*UU3/DK1/DKK
  H22C=N*XX*AJ1*UU6/DK1/DKK
  AAN7(II)=WET(II)*(G2DE*H21B-G2ED*H21C+G4DE*H22B-G4ED*H22C)
&*DEXP(DDK(II))
```

```
      CALL BEST(N,2,2,3,DKK,-BB,AW1)
      CALL BEST(N,0,0,3,DKK,-BB,AW2)
      CALL BEST(N,1,1,2,DKK,-BB,AW3)
      CALL BEST(N,2,2,3,DKK,CC,AW4)
      CALL BEST(N,0,0,3,DKK,CC,AW5)
      CALL BEST(N,1,1,2,DKK,CC,AW6)
      H23B=.5*XX*AJ1*(AW1-N*(N+1)*AW2/(-BB)**2.)/DKK**2./DK1
      H23C=.5*XX*AJ1*(AW4-N*(N+1)*AW5/CC**2.)/DKK**2./DK1
      H24B=XX*AJ1*AW3/DK1/DKK
      H24C=XX*AJ1*AW6/DK1/DKK
      AAN8(II)=WET(II)*(G2DE*H23B-G2ED*H23C+G4DE*H24B-G4ED*H24C)
     &*DEXP(DDK(II))
2001  CONTINUE
      SUM1=0.D0
      SUM2=0.D0
      SUM3=0.D0
      SUM4=0.D0
      SUM5=0.D0
      SUM6=0.D0
      SUM7=0.D0
      SUM8=0.D0
      SUM9=0.D0

      DO 1999 IJ=1,IN
      SUM1=SUM1+AAN(IJ)
      SUM2=SUM2+AAN1(IJ)
      SUM3=SUM3+AAN2(IJ)
      SUM4=SUM4+AAN3(IJ)
      SUM5=SUM5+AAN4(IJ)
      SUM6=SUM6+AAN5(IJ)
      SUM7=SUM7+AAN6(IJ)
      SUM8=SUM8+AAN7(IJ)
      SUM9=SUM9+AAN8(IJ)
1999  CONTINUE
      RETURN
      END

      SUBROUTINE BEST(N,M,J,L,ABK,ZZ1,BBB)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PI=DACOS(-1.D0)
      FFD=0.D0
      DO 104 IQ=0,N/2
      CALL GAMMA(N-2*IQ-M,AA1)
      CALL GAMMA(IQ,AA2)
      XZ=ABK*ABS(ZZ1)
      CALL AKV(N,IQ,J,XZ,WK)
      FFD1=((2/PI)**.5)/((-2.D0)**IQ)/AA2/AA1/(ZZ1)**(N+M)
      IF (N-2*IQ-M .LT. 0) THEN
      FFD1=0.D0
      END IF
      FFD=FFD+FFD1*WK*(ABK*ABS(ZZ1))**(N-IQ+L-.5)
104   CONTINUE
      BBB=FFD
      IF (N .LT. M) THEN
      BBB=0.D0
      END IF
      RETURN
      END
```

```
      SUBROUTINE AKV(N,IQ,J,X,FDK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION AAK(-20:80),FFK(-20:80)
      IF (N-IQ-J .GE. 1) THEN
      NN=N-IQ-J-1
      ELSE
      NN=N-IQ-J
      END IF
      PI=DACOS(-1.D0)
      AAK(0)=-1.*(.5D0*PI/X)/DEXP(X)
      AAK(1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      AAK(-1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(-2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(0)=(.5D0*PI/X)**.5/DEXP(X)
      FFK(1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(-1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(-2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      IF (IABS(NN) .LE. 2 ) THEN
      GO TO 2233
      END IF
      DO 502 I=3,IABS(NN)
      AAK(I)=AAK(I-2)-(2*I-1)*AAK(I-1)/X
      FFK(I)=AAK(I)/(-1.)**(I+1)/(.5*PI/X)**.5
      FFK(-I)=FFK(I)
502   CONTINUE
2233  CONTINUE
      FDK=FFK(NN)
4443  CONTINUE
      RETURN
      END

      SUBROUTINE GAMMA(J,AJK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IF (J .LE. 0) THEN
      AJK=1.D0
      ELSE
      AJK=1.D0
      DO 300 I=1,J
      SS=DBLE(I)
      AJK=AJK*SS
300   CONTINUE
      END IF
      RETURN
      END

      SUBROUTINE BESSEL(X,AJ0,AJ1,AJ2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      AJ0=0.D0
      AJ1=0.D0
      AJ2=0.D0
      DO 100 J=0,50
      CALL GAMMA(J,AJK)
      TJ=AJ0
      AJ0=AJ0+((-1.D0)**J)*(X/2)**(2*J)/(AJK)**2.
      IF (ABS(AJ0-TJ) .LE. 0.000000000000001 ) THEN
```

```
      GO TO 500
      END IF
100   CONTINUE
500   CONTINUE
      DO 107 J=0,50
      CALL GAMMA(J,AJK)
      TJ1=AJ1
      AJ1=AJ1+((-1.D0)**J)*(X/2)**(2*J+1)/((AJK)**2.)/(J+1)
      IF (ABS(AJ1-TJ1) .LE. 0.000000000000001 ) THEN
      GO TO 201
      END IF
107   CONTINUE
201   CONTINUE
      DO 108 J=0,50
      CALL GAMMA(J,AJK)
      TJ2=AJ2
      AJ2=AJ2+((-1.D0)**J)*(X/2.)**(2*J+2)/((AJK)**2.)/(J+1)
     &/(J+2)
      IF (ABS(AJ2-TJ2)    .LE. 0.0000000000000001) THEN
      GO TO 200
      END IF
108   CONTINUE
200   CONTINUE
      RETURN
      END

      SUBROUTINE FU(I,J,K,X,RAD,PI,U2,U3,R2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION RAD(2)
      INTEGER X
      PID=1.D-3
      DTHETA=(PI-4.D0*PID)/(X-2)
      IF(J==1) THEN
      Z=RAD(I)*DCOS(PID)
      V=RAD(I)*DSIN(PID)
      END IF
      IF((1<J) .AND. (J<=X/2)) THEN
      Z=RAD(I)*DCOS(PID+(J-1)*DTHETA)
      V=RAD(I)*DSIN(PID+(J-1)*DTHETA)
      END IF
      IF(X/2<J) THEN
      Z=RAD(I)*DCOS(PI/2.D0+(J-1-X/2)*DTHETA)
      V=RAD(I)*DSIN(PI/2.D0+(J-1-X/2)*DTHETA)
      END IF
      U2=Z/RAD(I)
      U3=V/RAD(I)
      R2=RAD(I)
      RETURN
      END

      SUBROUTINE GAUSL (N,M,II,JJ,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(N,M)
      DO 10 I=1,II
      AA=0.E0
      DO 9 J=1,II
9     AA=AA+ABS(A(I,J))
      DO 10 J=1,JJ
```

```
10      A(I,J)=A(I,J)/AA
        CALL XXXXX (N,M,II,JJ-II,A)
        RETURN
        END

        SUBROUTINE XXXXX (ND,NCOL,N,NS,A)
        IMPLICIT REAL*8 (A-H,O-Z)
        DIMENSION A(ND,NCOL)
        N1=N+1
        NT=N+NS
        IF(N.EQ.1) GO TO 50
        DO 10 I=2,N
        IP=I-1
        I1=IP
        X=ABS(A(I1,I1))
        DO 11 J=I,N
        IF(ABS(A(J,I1)).LT.X) GO TO 11
        X=ABS(A(J,I1))
        IP=J
11      CONTINUE
        IF(IP.EQ.I1) GO TO 13
        DO 12 J=I1,NT
        X=A(I1,J)
        A(I1,J)=A(IP,J)
12      A(IP,J)=X
13      DO 10 J=I,N
        X=A(J,I1)/A(I1,I1)
        DO 10 K=I,NT
10      A(J,K)=A(J,K)-X*A(I1,K)
50      DO 20 IP=1,N
        I=N1-IP
        DO 20 K=N1,NT
        A(I,K)=A(I,K)/A(I,I)
        IF(I.EQ.1) GO TO 20
        I1=I-1
        DO 25 J=1,I1
25      A(J,K)=A(J,K)-A(I,K)*A(J,I)
20      CONTINUE
        RETURN
        END

        SUBROUTINE FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
        IMPLICIT REAL*8 (A-H,O-Z)
        DIMENSION PA(-1:600)
        PA(-1)=0.D0
        PA(0)=0.D0
        PA(1)=(1.-U2**2)**.5
        PA(2)=3.*U2*(1.-U2**2)**.5
        DO 100 J=1,N+1
        PA(J+1)=((2*J+1)*U2*PA(J)-(J+1)*PA(J-1))/(J)
100     CONTINUE
        W1=PA(N)
        WW1=PA(N-1)
        WWW1=PA(N+1)
        PW1=(N*U2*PA(N)-(N+1)*PA(N-1))/(U2**2.-1.)
        PWW1=((N-1)*U2*PA(N-1)-(N)*PA(N-2))/(U2**2.-1.)
        PWWW1=((N+1)*U2*PA(N+1)-(N+2)*PA(N))/(U2**2.-1.)
        RETURN
```

```
      END

      SUBROUTINE FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION PR(-1:600)
      PR(-1)=0.D0
      PR(0)=1.D0
      PR(1)=U2
      DO 34 I=2,N+1
      PR(I)=((2*I-1)*U2*PR(I-1)-(I-1)*PR(I-2))/I
34    CONTINUE
      W=PR(N)
      WW=PR(N-1)
      WWW=PR(N+1)
      PW=(N*U2*PR(N)-N*PR(N-1))/(U2**2.-1.)
      PWW=((N-1)*U2*PR(N-1)-(N-1)*PR(N-2))/(U2**2.-1.)
      PWWW=((N+1)*U2*PR(N+1)-(N+1)*PR(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION PB(-1:600)
      PB(-1)=0.D0
      PB(0)=0.D0
      PB(1)=0.D0
      PB(2)=3.*(1.-U2**2)
      DO 150 K=2,N+1
      PB(K+1)=((2*K+1)*U2*PB(K)-(K+2)*PB(K-1))/(K-1)
150   CONTINUE
      W2=PB(N)
      WW2=PB(N-1)
      WWW2=PB(N+1)
      PW2=(N*U2*PB(N)-(N+2)*PB(N-1))/(U2**2.-1.)
      PWW2=((N-1)*U2*PB(N-1)-(N+1)*PB(N-2))/(U2**2.-1.)
      PWWW2=((N+1)*U2*PB(N+1)-(N+3)*PB(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,
     &DDK,WET,SM0,SM1,SM2,SM3,SM4)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN4(96),RAD(2),AN1(96),AN2(96),AN3(96)
      DIMENSION AN0(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      E2=DDK(II)*(ZZ-CC)
      E1=DDK(II)*(BB+CC)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      DK2=DKK*RAD(1)*U2
      CALL BESSEL(DK,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      PAJ0=-AJ1
```

```
      AJ3=4*AJ2/DK-AJ1
      PPAJ1=(-3*AJ1/4+AJ3/4)
      CALL BEST(N+1,1,1,0,DKK,-BB,VV1)
      CALL BEST (N+1,1,1,0,DKK,CC,VV2)
      AN0(II)=WET(II)*N*(U4)*((CC)**2.*DCOSH(E3)*AJ1*VV2/DSINH(E1)-
     &(-BB)**2.*AJ1*VV1*DCOSH(E2)/DSINH(E1))*DEXP(DKK)
      AN1(II)=WET(II)*N*(DKK*CC**2.*U2*DSINH(E3)*AJ1*U4*VV2/DSINH(
     &E1)+DKK*CC**2.*U3*DCOSH(E3)*PAJ1*VV2*U4/DSINH(E1)-DKK*
     &(-BB)**2.*U2*DSINH(E2)*AJ1*VV1*U4/DSINH(E1)-DKK*(-BB)**2.*U3
     &*DCOSH(E2)*PAJ1*VV1*U4/DSINH(E1))*DEXP(DKK)
      AN2(II)=WET(II)*N*
     &((DKK*U3)**2*(CC**2.*DCOSH(E3)*PPAJ1*U4*VV2/DSINH(E1)
     &-(-BB)**2.*DCOSH(E2)*PPAJ1*VV1*U4/DSINH(E1))
     &+2*(PAJ1*DKK*U3*(DKK*CC**2.*U2*DSINH(E3)*U4*VV2
     &-DKK*(-BB)**2.*U2*DSINH(E2)*VV1*U4)/DSINH(E1))
     &+AJ1*(DKK*U2)**2*(CC**2.*DCOSH(E3)*VV2*U4/DSINH(E1)
     &-(-BB)**2.*DCOSH(E2)*VV1*U4/DSINH(E1)))*DEXP(DKK)
      AN3(II)=WET(II)*N*(-DKK*CC**2.*RAD(1)*U3*DSINH(E3)*AJ1*U4*VV2/
     &DSINH(E1)+DKK*CC**2.*RAD(1)*U2*DCOSH(E3)*PAJ1*VV2*U4/DSINH
     &(E1)+DKK*(-BB)**2.*RAD(1)*U3*DSINH(E2)*AJ1*VV1*U4/DSINH(E1)-
     &DKK*(-BB)**2.*RAD(1)*U2*DCOSH(E2)*PAJ1*VV1*U4/DSINH(E1))*
     &DEXP(DKK)
      AN4(II)=WET(II)*N*(-1*U5)*((CC)**2.*DCOSH(E3)*AJ1*VV2/DSINH(E1)-
     &(-BB)**2.*AJ1*VV1*DCOSH(E2)/DSINH(E1))*DEXP(DKK)
2001  CONTINUE

      SM0=0.D0
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      SM4=0.D0
      DO 1999 IJ=1,IN
      SM0=SM0+AN0(IJ)
      SM1=SM1+AN1(IJ)
      SM2=SM2+AN2(IJ)
      SM3=SM3+AN3(IJ)
      SM4=SM4+AN4(IJ)
1999  CONTINUE
      RETURN
      END

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                 FOR LINEAR CONCENTRATION PROFILE                    C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

      SUBROUTINE XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM0,SM1,SM2
```

```
     &,SM3,SM4)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN4(96),RAD(2),AN1(96),AN2(96),AN3(96)
      DIMENSION AN0(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      E2=DDK(II)*(ZZ-CC)
      E1=DDK(II)*(BB+CC)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      DK2=DKK*RAD(1)*U2
      CALL BESSEL(DK,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      PAJ0=-AJ1
      AJ3=4*AJ2/DK-AJ1
      PPAJ1=(-3*AJ1/4+AJ3/4)
      CALL BEST(N,1,1,0,DKK,-BB,VV1)
      CALL BEST(N,1,1,0,DKK,CC,VV2)
      AN0(II)=WET(II)*(-DKK)*(U4)*((CC)**2.*DSINH(E3)*AJ1*VV2/DSINH(E1)
     &-(-BB)**2.*AJ1*VV1*DSINH(E2)/DSINH(E1))*DEXP(DKK)
      AN1(II)=WET(II)*(-DKK)*(DKK*CC**2.*U2*DCOSH(E3)*AJ1*U4*VV2/DSINH(
     & E1)+DKK*CC**2.*U3*DSINH(E3)*PAJ1*VV2*U4/DSINH(E1)-DKK*
     & (-BB)**2.*U2*DCOSH(E2)*AJ1*VV1*U4/DSINH(E1)-DKK*(-BB)**2.*U3
     & *DSINH(E2)*PAJ1*VV1*U4/DSINH(E1))*DEXP(DKK)
      AN2(II)=WET(II)*(-DKK)*
      &((DKK*U3)**2*(CC**2.*DSINH(E3)*PPAJ1*U4*VV2/DSINH(E1)
     &-(-BB)**2.*DSINH(E2)*PPAJ1*VV1*U4/DSINH(E1))
     &+2*(PAJ1*DKK*U3*(DKK*CC**2.*U2*DCOSH(E3)*U4*VV2
     &-DKK*(-BB)**2.*U2*DCOSH(E2)*VV1*U4)/DSINH(E1))
     &+AJ1*(DKK*U2)**2*(CC**2.*DSINH(E3)*VV2*U4/DSINH(E1)
     &-(-BB)**2.*DSINH(E2)*VV1*U4/DSINH(E1)))*DEXP(DKK)
      AN3(II)=WET(II)*(-DKK)*(-DKK*CC**2.*RAD(1)*U3*DCOSH(E3)*AJ1
     &*U4*VV2/DSINH(E1)+DKK*CC**2.*RAD(1)*U2*DSINH(E3)*PAJ1*VV2*U4
     &/DSINH(E1)+DKK*(-BB)**2.*RAD(1)*U3*DCOSH(E2)*AJ1*VV1*U4/DSINH(E1)-
     &DKK*(-BB)**2.*RAD(1)*U2*DSINH(E2)*PAJ1*VV1*U4/DSINH(E1))*
     & DEXP(DKK)
      AN4(II)=WET(II)*(-DKK)*(-1*U5)*((CC)**2.*DSINH(E3)*AJ1*VV2
     &/DSINH(E1)-(-BB)**2.*AJ1*VV1*DSINH(E2)/DSINH(E1))*DEXP(DKK)
2001  CONTINUE
      SM0=0.D0
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      SM4=0.D0
      DO 1999 IJ=1,IN
      SM0=SM0+AN0(IJ)
      SM1=SM1+AN1(IJ)
      SM2=SM2+AN2(IJ)
      SM3=SM3+AN3(IJ)
      SM4=SM4+AN4(IJ)
1999  CONTINUE
      RETURN
      END
```

Appendix E3-1: Computer programming source code for estimating the thermocapillary velocity of one spherical drop parallel one insulated plate.

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(500,501),RAD(2),DDK(96),WET(96),B(500,501),BF(500,3)
      INTEGER T,GG,LL1,LL2,LBB,LCC,GGG
      OPEN (23,FILE='GAUSS.DAT',STATUS='OLD')
      OPEN (24,FILE='WET3.DAT',STATUS='OLD')
      OPEN (25,FILE='DTTH0-10.DAT',STATUS='NEW')
      IN=40
      ETK=0.D0
      ETA=10.D0
      BB=.1D0
      DO 1001 I=1,IN
      READ (23,*) DDK(I),WET(I)
1001  CONTINUE
      T=1
      PI=DACOS(-1.D0)
      FI=.01*PI/180.
      U4=DCOS(FI)
      U5=DSIN(FI)
      DO 3231    IUY=1,50
      READ (24,*) CV,NX
      RAD(1)=CV*BB
      GGG=2*NX
      DO 511 I=1,T
      DO 512 J=1,NX
      NU=J+NX*(I-1)
      NY=J+NX*(I-1)+T*NX
      DO 513 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      B(NU,GGG+1)=-1.*RAD(1)*U3
      B(NY,GGG+1)=-1.*U3
      DO 514 N=1,NX
      NZ=(2*N-1)+2*NX*(K-1)
      NL=2*N+2*NX*(K-1)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      B(NU,NZ)=R2**(-N-1)*W1+SM1
      B(NU,NL)=-R2**N*W1
      B(NY,NZ)=(-N-1)*R2**(-N-2)*W1+SM2
      B(NY,NL)=-ETK*N*R2**(N-1)*W1

514   CONTINUE
513   CONTINUE
512   CONTINUE
511   CONTINUE

      LL1=500
      LL2=501
      LBB=GGG
      LCC=GGG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,B)
      GG=T*NX
      DO 7765 NN=1,2
```

```
      DO 111 I=1,T
      DO 112 J=1,NX
      NO=J+NX*(I-1)
      NP=J+NX*(I-1)+T*NX
      NQ=J+NX*(I-1)+2*T*NX
      NR=J+NX*(I-1)+3*T*NX
      NS=J+NX*(I-1)+4*T*NX
      NT=J+NX*(I-1)+5*T*NX
      DO 113 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      IF (NN .EQ. 1) THEN
      A(NO,6*GG+1)=U3*U4
      A(NP,6*GG+1)=0.D0
      A(NQ,6*GG+1)=0.D0
      A(NR,6*GG+1)=0.D0
      A(NS,6*GG+1)=0.D0
      A(NT,6*GG+1)=0.D0
      END IF
      DO 114 N=1,NX
      NE=(6*N-5)+6*NX*(K-1)
      NF=(6*N-4)+6*NX*(K-1)
      NG=(6*N-3)+6*NX*(K-1)
      NH=(6*N-2)+6*NX*(K-1)
      NI=(6*N-1)+6*NX*(K-1)
      NJ=(6*N-0)+6*NX*(K-1)
      CALL FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
      CALL XXD(FI,N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SUM1,SUM2,SUM3
     &,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9,SUM10,SUM11,SUM12,SUM13,SUM14
     &,SUM17,SUM18,SUM19,SUM20,SUM21,SUM22,SUM23,SUM24,SUM25,SUM26,
     & SUM27,SUM28,SUM29,SUM30,SUM31,SUM32,SUM33,SUM34,SUM35,SUM36
     & ,SUM15,SUM16)
      AA1=((2.*N*(2*N-1)*U3*W1*U4**2.+(N-2)*WW2*DCOS(2.*FI)-N*(N+1)
     * *(N-2)*WW)/2./R2**(N))
      BB1=-1.*(WWW2*DCOS(2.*FI)-N*(N+1)*WWW)/2./R2**(N+2)
      CC1=(W2*DCOS(2.*FI)+N*(N+1)*W)/2./R2**(N+1)
      AA2=(N*(2*N-1)*U3*W1+(N-2)*WW2)*U4*U5/R2**(N)
      BB2=-1.*(WWW2*U4*U5)/R2**(N+2)
      CC2=(W2*U4*U5)/R2**(N+1)
      AA3=(N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U4/R2**N
      BB3=-1.*(N*WWW1*U4)/R2**(N+2)
      CC3=-1.*(W1*U4)/R2**(N+1)
      AA1R=-1.*N*AA1/R2
      BB1R=-1.*(N+2)*BB1/R2
      CC1R=-1.*(N+1)*CC1/R2
      AA2R=-1.*N*AA2/R2
      BB2R=-1.*(N+2)*BB2/R2
      CC2R=-1.*(N+1)*CC2/R2
      AA3R=-1.*N*AA3/R2
      BB3R=-1.*(N+2)*BB3/R2
      CC3R=-1.*(N+1)*CC3/R2
      AA1S=(2.*N*(2*N-1)*U2*W1*U4**2.-2.*N*(2*N-1)*U3**2.*PW1*U4**2.-
     *    (N-2)*U3*PWW2*DCOS(2.*FI)+N*(N+1)*(N-2)*U3*PWW)/2./R2**N
      BB1S=-1.*(-1.*U3*PWWW2*DCOS(2.*FI)+N*(N+1)*U3*PWWW)/2./R2**(N+2)
      CC1S=(-1.*U3*PW2*DCOS(2.*FI)-U3*N*(N+1)*PW)/2./R2**(N+1)
      AA2S=(U2*N*(2*N-1)*W1-N*(2*N-1)*U3**2.*PW1-U3*(N-2)*PWW2)*U4*
     &U5/R2**N
```

```
  BB2S=(U3*PWWW2*U4*U5)/R2**(N+2)
  CC2S=(-1.*U3*PW2*U4*U5)/R2**(N+1)
  AA3S=(-1.*N*(2.*N-1)*U3*W1-U2*U3*N*(2*N-1)*PW1+U3*(N+1)*(N-2)
&*PWW1)*U4/R2**N
  BB3S=U3*N*PWWW1*U4/R2**(N+2)
  CC3S=U3*PW1*U4/R2**(N+1)
  AA1F=((-2.*N*(2*N-1)*U3*W1*U4*U5-(N-2)*WW2*DSIN(2.*FI)
* )/R2**(N))
  BB1F=WWW2*DSIN(2.*FI)/R2**(N+2)
  CC1F=-1.*W2*DSIN(2.*FI)/R2**(N+1)
  AA2F=(N*(2*N-1)*U3*W1+(N-2)*WW2)*DCOS(2.*FI)/R2**(N)
  BB2F=-1.*(WWW2*DCOS(2.*FI))/R2**(N+2)
  CC2F=(W2*DCOS(2.*FI))/R2**(N+1)
  AA3F=-1.*(N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U5/R2**N
  BB3F=(N*WWW1*U5)/R2**(N+2)
  CC3F=(W1*U5)/R2**(N+1)
  A(NO,NE)=U3*U4*(AA1+SUM1)+U3*U5*(AA2+SUM2)+U2*(AA3+SUM3)
  A(NO,NG)=U3*U4*(BB1+SUM4)+U3*U5*(BB2+SUM5)+U2*(BB3+SUM6)
  A(NO,NI)=U3*U4*(CC1+SUM7)+U3*U5*(CC2+SUM8)+U2*(CC3+SUM9)
  A(NO,NF)=0.D0
  A(NO,NH)=0.D0
  A(NO,NJ)=0.D0
  A(NP,NE)=U3*U4*(AA1+SUM1)+U3*U5*(AA2+SUM2)+U2*(AA3+SUM3)
  A(NP,NG)=U3*U4*(BB1+SUM4)+U3*U5*(BB2+SUM5)+U2*(BB3+SUM6)
  A(NP,NI)=U3*U4*(CC1+SUM7)+U3*U5*(CC2+SUM8)+U2*(CC3+SUM9)
  A(NP,NF)=0.D0
  A(NP,NH)=-N*R2**(N-1)*W1*U4
  A(NP,NJ)=-N*R2**(N+1)*W1*U4/2./ETA/(2*N+3)
  A(NQ,NE)=U2*U4*(AA1+SUM1)+U2*U5*(AA2+SUM2)-U3*(AA3+SUM3)
  A(NQ,NG)=U2*U4*(BB1+SUM4)+U2*U5*(BB2+SUM5)-U3*(BB3+SUM6)
  A(NQ,NI)=U2*U4*(CC1+SUM7)+U2*U5*(CC2+SUM8)-U3*(CC3+SUM9)
  A(NQ,NF)=-1.*R2**N*W1*U4/U3
  A(NQ,NH)=R2**(N-1)*PW1*U3*U4
  A(NQ,NJ)=(N+3)*R2**(N+1)*PW1*U4*U3/2./ETA/(2*N+3)/(N+1)
  A(NR,NE)=-1.*U5*(AA1+SUM1)+U4*(AA2+SUM2)
  A(NR,NG)=-1.*U5*(BB1+SUM4)+U4*(BB2+SUM5)
  A(NR,NI)=-1.*U5*(CC1+SUM7)+U4*(CC2+SUM8)
  A(NR,NF)=-1.*R2**N*PW1*U3*U5
  A(NR,NH)=R2**(N-1)*W1*U5/U3
  A(NR,NJ)=(N+3)*R2**(N+1)*W1*U5/U3/2./ETA/(2*N+3)/(N+1)
  A(NS,NE)=U2*U4*(AA1R+SUM10)+U2*U5*(AA2R+SUM11)-U3*(AA3R+SUM12)
& +(U3*U4*(AA1S+SUM19)+U3*U5*(AA2S+SUM20)+U2*(AA3S+SUM21))/R2
  A(NS,NG)=U2*U4*(BB1R+SUM13)+U2*U5*(BB2R+SUM14)-U3*(BB3R+SUM15)
& +(U3*U4*(BB1S+SUM22)+U3*U5*(BB2S+SUM23)+U2*(BB3S+SUM24))/R2
  A(NS,NI)=U2*U4*(CC1R+SUM16)+U2*U5*(CC2R+SUM17)-U3*(CC3R+SUM18)
& +(U3*U4*(CC1S+SUM25)+U3*U5*(CC2S+SUM26)+U2*(CC3S+SUM27))/R2
  A(NS,NF)=-1.*ETA*(N-1)*R2**(N-1)*W1*U4/U3
  A(NS,NH)=2.*ETA*(N-1)*R2**(N-2)*U3*U4*PW1
  A(NS,NJ)=ETA*N*(N+2)*R2**N*U3*U4*PW1/ETA/(N+1)/(2*N+3)
  A(NT,NE)=-1.*U5*(AA1R+SUM10)+U4*(AA2R+SUM11)+(U4*(AA1F+SUM28)+
&U5*(AA2F+SUM29)+U2*(AA3F+SUM30)/U3)/R2
  A(NT,NG)=-1.*U5*(BB1R+SUM13)+U4*(BB2R+SUM14)+(U4*(BB1F+SUM31)+
&U5*(BB2F+SUM32)+U2*(BB3F+SUM33)/U3)/R2
  A(NT,NI)=-1.*U5*(CC1R+SUM16)+U4*(CC2R+SUM17)+(U4*(CC1F+SUM34)+
&U5*(CC2F+SUM35)+U2*(CC3F+SUM36)/U3)/R2
  A(NT,NF)=-1.*ETA*(N-1)*R2**(N-1)*PW1*U5*U3
  A(NT,NH)=2.*ETA*(N-1)*R2**(N-2)*U5*W1/U3
  A(NT,NJ)=ETA*N*(N+2)*R2**N*U5*W1/ETA/U3/(N+1)/(2*N+3)
```

```
114     CONTINUE
113     CONTINUE
112     CONTINUE
111     CONTINUE

          IF (NN .EQ. 2) THEN
          DO 811 J=1,NX
          NO=J
          NP=J+NX
          NQ=J+2*NX
          NR=J+3*NX
          NS=J+4*NX
          NT=J+5*NX
          CALL FU(1,J,1,NX,RAD,PI,U2,U3,R2)
          VALUE=0.D0
          VALUE1=0.D0
          DO 713 KK=1,NX
          NZ=2*KK-1
          CALL FUCK2(U2,KK,W1,WW1,WWW1,PW1,PWW1,PWWW1)
          CALL XRD(KK,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
          VALUE=VALUE+B(NZ,GGG+1)*(R2**(-KK-1)*PW1*U4*(-1.*U3)+U4*SM3)
          VALUE1=VALUE1+B(NZ,GGG+1)*(R2**(-KK-1)*W1*(-1.*U5)-U5*SM1)
713       CONTINUE
          A(NO,6*GG+1)=0.D0
          A(NP,6*GG+1)=0.D0
          A(NQ,6*GG+1)=0.D0
          A(NR,6*GG+1)=0.D0
          A(NS,6*GG+1)=(RAD(1)*U2*U4+VALUE)/RAD(1)
          A(NT,6*GG+1)=(-1.*RAD(1)*U3*U5+VALUE1)/RAD(1)/U3
811       CONTINUE
            END IF

        LL1=500
        LL2=501
        LBB=6*GG
        LCC=6*GG+1
        CALL GAUSL (LL1,LL2,LBB,LCC,A)
        DO 999 I=1,6*GG
        BF(I,NN)=A(I,6*GG+1)
999     CONTINUE
7765    CONTINUE
        VVU=2.*RAD(1)/(2.+3.*ETA)/(2.+ETK)
        HGD=-1.*BF(1,2)/BF(1,1)/VVU
        WRITE (25,9) CV,HGD
        WRITE (*,9) CV,HGD
3231    CONTINUE
9       FORMAT (2(F12.5))
        STOP
        END

        SUBROUTINE FU(I,J,K,NX,RAD,PI,U2,U3,R2)
        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
        DIMENSION RAD(2)
        PID=1.D-3
        DTHETA=(PI-4.D0*PID)/(NX-2)
        IF(J==1) THEN
        Z=RAD(I)*DCOS(PID)
```

```
      V=RAD(I)*DSIN(PID)
      END IF
      IF((1<J) .AND. (J<=NX/2)) THEN
      Z=RAD(I)*DCOS(PID+(J-1)*DTHETA)
      V=RAD(I)*DSIN(PID+(J-1)*DTHETA)
      END IF
      IF(NX/2<J) THEN
      Z=RAD(I)*DCOS(PI/2.D0+(J-1-NX/2)*DTHETA)
      V=RAD(I)*DSIN(PI/2.D0+(J-1-NX/2)*DTHETA)
      END IF
      U2=Z/RAD(I)
      U3=V/RAD(I)
      R2=RAD(I)
      RETURN
      END

      SUBROUTINE GAUSL (N,M,II,JJ,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(N,M)
      DO 10 I=1,II
      AA=0.E0
      DO 9 J=1,II
    9 AA=AA+ABS(A(I,J))
      DO 10 J=1,JJ
   10 A(I,J)=A(I,J)/AA
      CALL XXXXX (N,M,II,JJ-II,A)
      RETURN
      END
      SUBROUTINE XXXXX (ND,NCOL,N,NS,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(ND,NCOL)
      N1=N+1
      NT=N+NS
      IF(N.EQ.1) GO TO 50
      DO 10 I=2,N
      IP=I-1
      I1=IP
      X=ABS(A(I1,I1))
      DO 11 J=I,N
      IF(ABS(A(J,I1)).LT.X) GO TO 11
      X=ABS(A(J,I1))
      IP=J
   11 CONTINUE
      IF(IP.EQ.I1) GO TO 13
      DO 12 J=I1,NT
      X=A(I1,J)
      A(I1,J)=A(IP,J)
   12 A(IP,J)=X
   13 DO 10 J=I,N
      X=A(J,I1)/A(I1,I1)
      DO 10 K=I,NT
   10 A(J,K)=A(J,K)-X*A(I1,K)
   50 DO 20 IP=1,N
      I=N1-IP
      DO 20 K=N1,NT
      A(I,K)=A(I,K)/A(I,I)
      IF(I.EQ.1) GO TO 20
      I1=I-1
```

```
      DO 25 J=1,I1
   25 A(J,K)=A(J,K)-A(I,K)*A(J,I)
   20 CONTINUE
      RETURN
      END

      SUBROUTINE FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PA(-1:600)
      PA(-1)=0.D0
      PA(0)=0.D0
      PA(1)=(1.-U2**2)**.5
      PA(2)=3.*U2*(1.-U2**2)**.5
      DO 100 J=1,N+1
      PA(J+1)=((2*J+1)*U2*PA(J)-(J+1)*PA(J-1))/(J)
100   CONTINUE
      W1=PA(N)
      WW1=PA(N-1)
      WWW1=PA(N+1)
      PW1=(N*U2*PA(N)-(N+1)*PA(N-1))/(U2**2.-1.)
      PWW1=((N-1)*U2*PA(N-1)-(N)*PA(N-2))/(U2**2.-1.)
      PWWW1=((N+1)*U2*PA(N+1)-(N+2)*PA(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PR(-1:600)
      PR(-1)=0.D0
      PR(0)=1.D0
      PR(1)=U2
      DO 34 I=2,N+1
      PR(I)=((2*I-1)*U2*PR(I-1)-(I-1)*PR(I-2))/I
34    CONTINUE
      W=PR(N)
      WW=PR(N-1)
      WWW=PR(N+1)
      PW=(N*U2*PR(N)-N*PR(N-1))/(U2**2.-1.)
      PWW=((N-1)*U2*PR(N-1)-(N-1)*PR(N-2))/(U2**2.-1.)
      PWWW=((N+1)*U2*PR(N+1)-(N+1)*PR(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PB(-1:600)
      PB(-1)=0.D0
      PB(0)=0.D0
      PB(1)=0.D0
      PB(2)=3.*(1.-U2**2)
      DO 150 K=2,N+1
      PB(K+1)=((2*K+1)*U2*PB(K)-(K+2)*PB(K-1))/(K-1)
150   CONTINUE
      W2=PB(N)
      WW2=PB(N-1)
      WWW2=PB(N+1)
      PW2=(N*U2*PB(N)-(N+2)*PB(N-1))/(U2**2.-1.)
      PWW2=((N-1)*U2*PB(N-1)-(N+1)*PB(N-2))/(U2**2.-1.)
```

```
  PWWW2=((N+1)*U2*PB(N+1)-(N+3)*PB(N))/(U2**2.-1.)
  RETURN
  END

  SUBROUTINE XXD(FI,N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SUM1,SUM2,SUM3
&,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9,SUM10,SUM11,SUM12,SUM13,SUM14
&,SUM17,SUM18,SUM19,SUM20,SUM21,SUM22,SUM23,SUM24,SUM25,SUM26,
& SUM27,SUM28,SUM29,SUM30,SUM31,SUM32,SUM33,SUM34,SUM35,SUM36
& ,SUM15,SUM16)
  IMPLICIT DOUBLE PRECISION (A-H,O-Z)
  DIMENSION WET(96),DDK(96),RAD(2)
  DIMENSION ANN1(96),ANN2(96),ANN3(96),BNN1(96),BNN2(96),BNN3(96)
  DIMENSION CNN1(96),CNN2(96),CNN3(96),ANN1R(96),ANN2R(96),ANN3R(96)
  DIMENSION BNN1R(96),BNN2R(96),BNN3R(96),CNN1R(96),CNN2R(96)
  DIMENSION CNN3R(96),ANN1S(96),ANN2S(96),ANN3S(96),BNN1S(96)
  DIMENSION BNN2S(96),BNN3S(96),CNN1S(96),CNN2S(96),CNN3S(96)
  DIMENSION ANN1F(96),ANN2F(96),ANN3F(96),BNN1F(96),BNN2F(96)
  DIMENSION BNN3F(96),CNN1F(96),CNN2F(96),CNN3F(96)
  DO 2001 II=1,IN
  Z=RAD(1)*U2
  X=RAD(1)*U3*U4
  Y=RAD(1)*U3*U5
  DKK=DDK(II)
  DY=RAD(1)*U3
  DDY=DKK*DY
  CALL BESSEL(DDY,AJ,AJ0,AJ1,AJ2)
  PAJ0=-1.*AJ1
  PAJ1=.5*(AJ0-AJ2)
  B1=AJ0*X**2.+(Y**2.-X**2.)*AJ1/DDY
  B2=(AJ0-2.*AJ1/DDY)/DDY**2.
  B1R=(X**2.*PAJ0*DDY+2.*X**2.*AJ0+(Y**2.-X**2.)*(AJ1+PAJ1*DDY)
& /DDY)/RAD(1)
  B1S=Z*(X**2.*PAJ0*DDY+2.*X**2.*AJ0+(Y**2.-X**2.)*(AJ1+PAJ1*DDY
& )/DDY)/DY
  B1F=-2.*X*Y*AJ0+4*X*Y*AJ1/DDY
  B2R=(6.*AJ1/DDY-2.*AJ0+DDY*PAJ0-2.*PAJ1)/RAD(1)/DDY**2.
  B2S=Z*(6.*AJ1/DDY-2.*AJ0+DDY*PAJ0-2.*PAJ1)/DDY**2./DY
  E3=DKK*(Z+BB)
  G5=DEXP(-1.*E3)
  G5R=-1.*DKK*U2*G5
  G5S=DKK*RAD(1)*U3*G5
  G6=-1.*E3*DEXP(-E3)
  G1=G6
  G6R=DKK*U2*(E3*G5-G5)
  G1R=G6R
  G6S=DKK*RAD(1)*U3*(G5-E3*G5)
  G1S=G6S
  G2=-1.*G6
  G2R=-1.*G6R
  G2S=-1.*G6S
  G3=(1.-E3)*G5
  G3R=DKK*U2*(E3*G5-2.*G5)
  G3S=DKK*RAD(1)*U3*(2.*G5-E3*G5)
  G4=(1.+E3)*G5
  G4R=-1.*DKK*U2*E3*G5
  G4S=DKK*RAD(1)*U3*E3*G5
  CALL BEST(N,1,1,0,DKK,-BB,F1)
  CALL BEST(N,1,2,1,DKK,-BB,F2)
```

```
  CALL BEST(N-1,2,2,3,DKK,-BB,F3)
  CALL BEST(N-1,0,0,1,DKK,-BB,F4)
  CALL BEST(N-1,2,2,1,DKK,-BB,F5)
  CALL BEST(N-1,1,1,0,DKK,-BB,F6)
  CALL BEST(N+1,2,2,3,DKK,-BB,F7)
  CALL BEST(N+1,0,0,1,DKK,-BB,F8)
  CALL BEST(N+1,2,2,1,DKK,-BB,F9)
  CALL BEST(N+1,1,1,0,DKK,-BB,F10)
  CALL BEST(N,2,2,3,DKK,-BB,F11)
  CALL BEST(N,0,0,1,DKK,-BB,F12)
  CALL BEST(N,2,2,1,DKK,-BB,F13)
  CALL BEST(N,1,1,2,DKK,-BB,F14)
  CALL BEST(N-1,0,0,3,DKK,-BB,F15)
  CALL BEST(N,1,2,3,DKK,-BB,F16)
  CALL BEST(N-1,1,1,2,DKK,-BB,F17)
  CALL BEST(N+1,0,0,3,DKK,-BB,F18)
  CALL BEST(N+1,1,1,2,DKK,-BB,F19)
  CALL BEST(N,0,0,3,DKK,-BB,F20)
  H1=-N*(2*N-1)*(-BB)**2.*AJ0*F1+N*(2*N-1)*(-BB)**2.*B1*F2/DY**2.-
& .5*(N-2)*(Y**2.-X**2.)*B2*F3+.5*N*(N+1)*(N-2)*AJ0*F4
  H1R=-N*(2*N-1)*(-BB)**2.*PAJ0*DKK*U3*F1-2.*N*(2*N-1)*U3*(-BB)**2.
& *B1*F2/DY**3.+N*(2*N-1)*(-BB)**2.*B1R*F2/DY**2.-(N-2)*(Y**2.-
& X**2.)*B2*F3/RAD(1)-.5*(N-2)*(Y**2.-X**2.)*B2R*F3+.5*N*(N+1)*(N-
& 2)*PAJ0*DKK*U3*F4
  H1S=-N*(2*N-1)*(-BB)**2.*PAJ0*DKK*RAD(1)*U2*F1-2.*N*(2*N-1)*U2*
& RAD(1)*(-BB)**2.*B1*F2/DY**3.+N*(2*N-1)*(-BB)**2.*B1S*F2/DY**2.
& -(N-2)*(Y**2.-X**2.)*B2*F3*Z/DY-.5*(N-2)*(Y**2.-X**2.)*B2S*F3
& +.5*N*(N+1)*(N-2)*DKK*RAD(1)*U2*F4*PAJ0
  H1F=N*(2*N-1)*(-BB)**2.*B1F*F2/DY**2.-2.*(N-2)*X*Y*B2*F3
  H2=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
& (N+1)*(N-2)*F4)*B1/DY**2.
  H2R=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
& (N+1)*(N-2)*F4)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H2S=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
& (N+1)*(N-2)*F4)*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H2F=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
& (N+1)*(N-2)*F4)*B1F/DY**2.
  H3=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*B1/DY**2.
  H3R=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*(B1R/
& DY**2.-2.*U3*B1/DY**3.)
  H3S=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*(B1S/
& DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H3F=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*B1F/
& DY**2.
  H4=.5*((Y**2.-X**2.)*B2*F7-N*(N+1)*AJ0*F8)
  H4R=.5*(2.*(Y**2.-X**2.)*B2*F7/RAD(1)+(Y**2.-X**2.)*B2R*F7-N*
& (N+1)*PAJ0*DKK*U3*F8)
  H4S=.5*(2.*Z*(Y**2.-X**2.)*B2*F7/DY+(Y**2.-X**2.)*B2S*F7-N*(N+1)
& *PAJ0*DKK*RAD(1)*U2*F8)
  H4F=2.*X*Y*B2*F7
  H5=-.5*((-BB)**2.*F9+N*(N+1)*F8)*B1/DY**2.
  H5R=-.5*((-BB)**2.*F9+N*(N+1)*F8)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H5S=-.5*((-BB)**2.*F9+N*(N+1)*F8)*(B1S/DY**2.-2.*RAD(1)*U2*B1/
& DY**3.)
  H5F=-.5*((-BB)**2.*F9+N*(N+1)*F8)*B1F/DY**2.
  H6=N*DKK*(-BB)**2.*B1*F10/DY**2.
  H6R=N*DKK*(-BB)**2.*F10*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H6S=N*DKK*(-BB)**2.*F10*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
```

```
  H6F=N*DKK*(-BB)**2.*F10*B1F/DY**2.
  H7=-.5*((Y**2.-X**2.)*B2*F11+N*(N+1)*AJ0*F12)
  H7R=-.5*(2.*(Y**2.-X**2.)*B2*F11/RAD(1)+(Y**2.-X**2.)*B2R*F11+N*
&    (N+1)*PAJ0*DKK*U3*F12)
  H7S=-.5*(2.*(Y**2.-X**2.)*Z*B2*F11/DY+(Y**2.-X**2.)*B2S*F11+N*
&    (N+1)*PAJ0*DKK*U2*RAD(1)*F12)
  H7F=-2.*X*Y*B2*F11
  H8=.5*((-BB)**2.*F13-N*(N+1)*F12)*B1/DY**2.
  H8R=.5*((-BB)**2.*F13-N*(N+1)*F12)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H8S=.5*((-BB)**2.*F13-N*(N+1)*F12)*(B1S/DY**2.-2.*U2*RAD(1)*B1/
&    DY**3.)
  H8F=.5*((-BB)**2.*F13-N*(N+1)*F12)*B1F/DY**2.
  H9=DKK*(-BB)**2.*F1*B1/DY**2.
  H9R=DKK*(-BB)**2.*F1*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H9S=DKK*(-BB)**2.*F1*(B1S/DY**2.-2.*U2*RAD(1)*B1/DY**3.)
  H9F=DKK*(-BB)**2.*F1*B1F/DY**2.
  H10=X*Y*B2*(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15
& /(-BB)**2.)
  H10R=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
& **2.)*(2.*X*Y*B2/RAD(1)+X*Y*B2R)
  H10S=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
& **2.)*(2.*Z*X*Y*B2/DY+X*Y*B2S)
  H10F=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
& **2.)*DY**2.*B2*DCOS(2.*FI)
  H11=X*Y*B2*(N*(2*N-1)*F16+(N-2)*F3)
  H11R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(N*(2*N-1)*F16+(N-2)*F3)
  H11S=(2.*Z*X*Y*B2/DY+X*Y*B2S)*(N*(2*N-1)*F16+(N-2)*F3)
  H11F=DY**2.*B2*DCOS(2.*FI)*(N*(2*N-1)*F16+(N-2)*F3)
  H12=DKK*X*Y*B2*(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)
  H12R=(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*(2.*X*Y*B2/RAD(1)
% +X*Y*B2R)*DKK
  H12S=(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*(2.*Z*X*Y*B2/DY
& +X*Y*B2S)*DKK
  H12F=DKK*(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*DY**2.*B2*
& DCOS(2.*FI)
  H13=.5*X*Y*B2*(F7-N*(N+1)*F18/(-BB)**2.)
  H13R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(F7-N*(N+1)*F18/(-BB)**2.)/2.
  H13S=(2.*X*Y*Z*B2/DY+X*Y*B2S)*(F7-N*(N+1)*F18/(-BB)**2.)/2.
  H13F=DY**2.*B2*DCOS(2.*FI)*(F7-N*(N+1)*F18/(-BB)**2.)/2.
  H14=-1.*X*Y*B2*F7
  H14R=-1.*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F7
  H14S=-1.*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F7
  H14F=-1.*DY**2.*B2*DCOS(2.*FI)*F7
  H15=N*DKK*X*Y*B2*F19
  H15R=N*DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F19
  H15S=N*DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F19
  H15F=N*DKK*DY**2.*B2*DCOS(2.*FI)*F19
  H16=-.5*X*Y*B2*(F11+N*(N+1)*F20/(-BB)**2.)
  H16R=-.5*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16S=-.5*(2.*X*Y*Z*B2/DY+X*Y*B2S)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16F=-.5*DY**2.*B2*DCOS(2.*FI)*(F11+N*(N+1)*F20/(-BB)**2.)
  H17=X*Y*B2*F11
  H17R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F11
  H17S=(2.*X*Y*Z*B2/DY+X*Y*B2S)*F11
  H17F=DY**2.*B2*DCOS(2.*FI)*F11
  H18=DKK*X*Y*B2*F14
  H18R=DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F14
  H18S=DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F14
```

```
  H18F=DKK*DY**2.*B2*DCOS(2.*FI)*F14
  H19=-1.*X*AJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*
&    F15/(-BB)**2.)/DKK**2./DY
  H19R=-1.*X*PAJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*
&    F15/(-BB)**2.)/DKK/RAD(1)
  H19S=-1.*X*Z*PAJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*
& (N-2)*F15/(-BB)**2.)/DKK/DY
  H19F=Y*AJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*F15
& /(-BB)**2.)/DKK**2./DY
  H20=-1.*X*AJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DKK/DY
  H20R=-1.*X*PAJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/RAD(1)
  H20S=-1.*X*Z*PAJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DY
  H20F=Y*AJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DY/DKK
  H21=-.5*X*AJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DKK**2./DY
  H21R=-.5*X*PAJ1*(F7+N*(N+1)*F18/(-BB)**2.)/RAD(1)/DKK
  H21S=-.5*X*Z*PAJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DY/DKK
  H21F=.5*Y*AJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DY/DKK**2.
  H22=N*X*AJ1*F19/DKK/DY
  H22R=N*X*PAJ1*F19/RAD(1)
  H22S=N*X*Z*PAJ1*F19/DY
  H22F=-1.*N*Y*AJ1*F19/DY/DKK
  H23=.5*X*AJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DKK**2./DY
  H23R=.5*X*PAJ1*(F11-N*(N+1)*F20/(-BB)**2.)/RAD(1)/DKK
  H23S=.5*X*Z*PAJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DY/DKK
  H23F=-.5*Y*AJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DY/DKK**2.
  H24=X*AJ1*F14/DKK/DY
  H24R=X*PAJ1*F14/RAD(1)
  H24S=X*Z*PAJ1*F14/DY
  H24F=-1.*Y*AJ1*F14/DY/DKK
  ANN1(II)=WET(II)*(G5*H1+G6*H2+G1*H3)*DEXP(DKK)
  ANN1R(II)=WET(II)*(G5R*H1+G5*H1R+G6R*H2+G6*H2R+G1R*H3+G1*H3R)
& *DEXP(DKK)
  ANN1S(II)=WET(II)*(G5S*H1+G5*H1S+G6S*H2+G6*H2S+G1S*H3+G1*H3S)
& *DEXP(DKK)
  ANN1F(II)=WET(II)*(G5*H1F+G6*H2F+G1*H3F)*DEXP(DKK)
  BNN1(II)=WET(II)*(G5*H4+G6*H5+G1*H6)*DEXP(DKK)
  BNN1R(II)=WET(II)*(G5R*H4+G5*H4R+G6R*H5+G6*H5R+G1R*H6+G1*H6R)
& *DEXP(DKK)
  BNN1S(II)=WET(II)*(G5S*H4+G5*H4S+G6S*H5+G6*H5S+G1S*H6+G1*H6S)
& *DEXP(DKK)
  BNN1F(II)=WET(II)*(G5*H4F+G6*H5F+G1*H6F)*DEXP(DKK)
  CNN1(II)=WET(II)*(G5*H7+G6*H8+G1*H9)*DEXP(DKK)
  CNN1R(II)=WET(II)*(G5R*H7+G5*H7R+G6R*H8+G6*H8R+G1R*H9+G1*H9R)
& *DEXP(DKK)
  CNN1S(II)=WET(II)*(G5S*H7+G5*H7S+G6S*H8+G6*H8S+G1S*H9+G1*H9S)
& *DEXP(DKK)
  CNN1F(II)=WET(II)*(G5*H7F+G6*H8F+G1*H9F)*DEXP(DKK)
  ANN2(II)=WET(II)*(G6*H10+G3*H11+G1*H12)*DEXP(DKK)
  ANN2R(II)=WET(II)*(G6R*H10+G6*H10R+G3R*H11+G3*H11R+G1R*H12+G1*
& H12R)*DEXP(DKK)
  ANN2S(II)=WET(II)*(G6S*H10+G6*H10S+G3S*H11+G3*H11S+G1S*H12+G1*
& H12S)*DEXP(DKK)
  ANN2F(II)=WET(II)*(G6*H10F+G3*H11F+G1*H12F)*DEXP(DKK)
  BNN2(II)=WET(II)*(G6*H13+G3*H14+G1*H15)*DEXP(DKK)
  BNN2R(II)=WET(II)*(G6R*H13+G6*H13R+G3R*H14+G3*H14R+G1R*H15+G1*
&    H15R)*DEXP(DKK)
  BNN2S(II)=WET(II)*(G6S*H13+G6*H13S+G3S*H14+G3*H14S+G1S*H15+G1*
&    H15S)*DEXP(DKK)
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```
      BNN2F(II)=WET(II)*(G6*H13F+G3*H14F+G1*H15F)*DEXP(DKK)
      CNN2(II)=WET(II)*(G6*H16+G3*H17+G1*H18)*DEXP(DKK)
      CNN2R(II)=WET(II)*(G6R*H16+G6*H16R+G3R*H17+G3*H17R+G1R*H18+G1*
     & H18R)*DEXP(DKK)
      CNN2S(II)=WET(II)*(G6S*H16+G6*H16S+G3S*H17+G3*H17S+G1S*H18+G1*
     & H18S)*DEXP(DKK)
      CNN2F(II)=WET(II)*(G6*H16F+G3*H17F+G1*H18F)*DEXP(DKK)
      ANN3(II)=WET(II)*(G2*H19+G4*H20)*DEXP(DKK)
      ANN3R(II)=WET(II)*(G2R*H19+G2*H19R+G4R*H20+G4*H20R)*DEXP(DKK)
      ANN3S(II)=WET(II)*(G2S*H19+G2*H19S+G4S*H20+G4*H20S)*DEXP(DKK)
      ANN3F(II)=WET(II)*(G2*H19F+G4*H20F)*DEXP(DKK)
      BNN3(II)=WET(II)*(G2*H21+G4*H22)*DEXP(DKK)
      BNN3R(II)=WET(II)*(G2R*H21+G2*H21R+G4R*H22+G4*H22R)*DEXP(DKK)
      BNN3S(II)=WET(II)*(G2S*H21+G2*H21S+G4S*H22+G4*H22S)*DEXP(DKK)
      BNN3F(II)=WET(II)*(G2*H21F+G4*H22F)*DEXP(DKK)
      CNN3(II)=WET(II)*(G2*H23+G4*H24)*DEXP(DKK)
      CNN3R(II)=WET(II)*(G2R*H23+G2*H23R+G4R*H24+G4*H24R)*DEXP(DKK)
      CNN3S(II)=WET(II)*(G2S*H23+G2*H23S+G4S*H24+G4*H24S)*DEXP(DKK)
      CNN3F(II)=WET(II)*(G2*H23F+G4*H24F)*DEXP(DKK)
2001  CONTINUE
      SUM1=0.D0
      SUM2=0.D0
      SUM3=0.D0
      SUM4=0.D0
      SUM5=0.D0
      SUM6=0.D0
      SUM7=0.D0
      SUM8=0.D0
      SUM9=0.D0
      SUM10=0.D0
      SUM11=0.D0
      SUM12=0.D0
      SUM13=0.D0
      SUM14=0.D0
      SUM15=0.D0
      SUM16=0.D0
      SUM17=0.D0
      SUM18=0.D0
      SUM19=0.D0
      SUM20=0.D0
      SUM21=0.D0
      SUM22=0.D0
      SUM23=0.D0
      SUM24=0.D0
      SUM25=0.D0
      SUM26=0.D0
      SUM27=0.D0
      SUM28=0.D0
      SUM29=0.D0
      SUM30=0.D0
      SUM31=0.D0
      SUM32=0.D0
      SUM33=0.D0
      SUM34=0.D0
      SUM35=0.D0
      SUM36=0.D0
      DO 1999 IJ=1,IN
      SUM1=SUM1+ANN1(IJ)
```

```
      SUM2=SUM2+ANN2(IJ)
      SUM3=SUM3+ANN3(IJ)
      SUM4=SUM4+BNN1(IJ)
      SUM5=SUM5+BNN2(IJ)
      SUM6=SUM6+BNN3(IJ)
      SUM7=SUM7+CNN1(IJ)
      SUM8=SUM8+CNN2(IJ)
      SUM9=SUM9+CNN3(IJ)
      SUM10=SUM10+ANN1R(IJ)
      SUM11=SUM11+ANN2R(IJ)
      SUM12=SUM12+ANN3R(IJ)
      SUM13=SUM13+BNN1R(IJ)
      SUM14=SUM14+BNN2R(IJ)
      SUM15=SUM15+BNN3R(IJ)
      SUM16=SUM16+CNN1R(IJ)
      SUM17=SUM17+CNN2R(IJ)
      SUM18=SUM18+CNN3R(IJ)
      SUM19=SUM19+ANN1S(IJ)
      SUM20=SUM20+ANN2S(IJ)
      SUM21=SUM21+ANN3S(IJ)
      SUM22=SUM22+BNN1S(IJ)
      SUM23=SUM23+BNN2S(IJ)
      SUM24=SUM24+BNN3S(IJ)
      SUM25=SUM25+CNN1S(IJ)
      SUM26=SUM26+CNN2S(IJ)
      SUM27=SUM27+CNN3S(IJ)
      SUM28=SUM28+ANN1F(IJ)
      SUM29=SUM29+ANN2F(IJ)
      SUM30=SUM30+ANN3F(IJ)
      SUM31=SUM31+BNN1F(IJ)
      SUM32=SUM32+BNN2F(IJ)
      SUM33=SUM33+BNN3F(IJ)
      SUM34=SUM34+CNN1F(IJ)
      SUM35=SUM35+CNN2F(IJ)
      SUM36=SUM36+CNN3F(IJ)
1999  CONTINUE
      RETURN
      END

      SUBROUTINE BEST(N,M,J,L,ABK,ZZ1,BBB)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PI=DACOS(-1.D0)
      FFD=0.D0
      DO 104 IQ=0,INT(N/2)
      IF (N-2*IQ-M .LT. 0) THEN
      FFD1=0.D0
      GO TO 1435
      ELSE
      CALL GAMMA(N-2*IQ-M,AA1)
      CALL GAMMA(IQ,AA2)
      XZ=ABK*ABS(ZZ1)
      FFD1=((2/PI)**.5)/((-2.D0)**IQ)/AA2/AA1/(ZZ1)**(N+M)
      END IF
      CALL AKV(N,IQ,J,XZ,WK)
1435  CONTINUE
      FFD=FFD+FFD1*WK*(ABK*ABS(ZZ1))**(N-IQ+L-.5)
104   CONTINUE
      BBB=FFD
```

```
      IF (N .LT. M) THEN
      BBB=0.D0
      END IF
      RETURN
      END

        SUBROUTINE AKV(N,IQ,J,X,FDK)
        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
        DIMENSION AAK(-20:80),FFK(-20:80)
        IF (N-IQ-J .GE. 1) THEN
        NN=N-IQ-J-1
        ELSE
        NN=N-IQ-J
        END IF
        PI=DACOS(-1.D0)
        AAK(0)=-1.*(.5D0*PI/X)/DEXP(X)
        AAK(1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
        AAK(2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
        AAK(-1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
        AAK(-2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
        FFK(0)=(.5D0*PI/X)**.5/DEXP(X)
        FFK(1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
        FFK(2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
        FFK(-1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
        FFK(-2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
        IF (IABS(NN) .LE. 2 ) THEN
        GO TO 2233
        END IF
        DO 502 I=3,IABS(NN)
        AAK(I)=AAK(I-2)-(2*I-1)*AAK(I-1)/X
        FFK(I)=AAK(I)/(-1.)**(I+1)/(.5*PI/X)**.5
        FFK(-I)=FFK(I)
502     CONTINUE
2233    CONTINUE
        FDK=FFK(NN)
4443    CONTINUE
        RETURN
        END

      SUBROUTINE GAMMA(J,AJK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IF (J .EQ. 0) THEN
      AJK=1.D0
      ELSE
      AJK=1.D0
      DO 300 I=1,J
      SS=DBLE(I)
      AJK=AJK*SS
300   CONTINUE
      END IF
      RETURN
      END

      SUBROUTINE BESSEL(CX,AJ,AJ0,AJ1,AJ2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      AJ0=0.D0
      AJ1=0.D0
      AJ2=0.D0
```

```
      DO 100 J=0,50
      CALL GAMMA(J,AJK)
      TJ=AJ0
      AJ0=AJ0+((-1.D0)**J)*(CX/2.)**(2*J)/(AJK)**2.
      IF (ABS(AJ0-TJ) .LE. 0.000000000000001 ) THEN
      GO TO    500
      END IF
100   CONTINUE
500   CONTINUE
      DO 107 J=0,50
      CALL GAMMA(J,AJK)
      TJ1=AJ1
      AJ1=AJ1+((-1.D0)**J)*(CX/2.)**(2*J+1)/((AJK)**2.)/(J+1)
      IF (ABS(AJ1-TJ1) .LE. 0.000000000000001 ) THEN
      GO TO 201
      END IF
107   CONTINUE
201   CONTINUE
      DO 108 J=0,50
      CALL GAMMA(J,AJK)
      TJ2=AJ2
      AJ2=AJ2+((-1.D0)**J)*(CX/2.)**(2*J+2)/((AJK)**2.)/(J+1)
     &/(J+2)
      IF (ABS(AJ2-TJ2)    .LE. 0.0000000000000001) THEN
      GO TO 200
      END IF
108   CONTINUE
200   CONTINUE
        AJ=-1.*AJ1
        RETURN
        END

      SUBROUTINE XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN(96),RAD(2),AN1(96),AN2(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=-1.*DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      CALL BEST(N+1,1,1,0,DKK,-BB,VV1)
      AN(II)=WET(II)*N*(-(BB)**2.*DEXP(E3)*AJ1*VV1)*DEXP(DDK(II))
      AN1(II)=WET(II)*N*(DKK*U2*DEXP(E3)*(BB)**2.*AJ1*VV1-DKK
     & *DEXP(E3)*(BB)**2.*PAJ1*U3*VV1)*DEXP(DKK)
      AN2(II)=WET(II)*N*(-DKK*RAD(1)*U3*DEXP(E3)*(BB)**2.*VV1*AJ1
     & -DKK*RAD(1)*U2*DEXP(E3)*(-BB)**2.*VV1*PAJ1)*DEXP(DKK)
2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN(IJ)
      SM2=SM2+AN1(IJ)
```

```
      SM3=SM3+AN2(IJ)
1999  CONTINUE
      RETURN
      END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                FOR LINEAR TEMPERATURE PROFILE                C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

```
      SUBROUTINE XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN(96),RAD(2),AN1(96),AN2(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=-1.*DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      CALL BEST(N,1,1,0,DKK,-BB,VV1)
      AN(II)=WET(II)*(-1.*DKK*(BB)**2.*DEXP(E3)*AJ1*VV1)*DEXP(DDK(II))
      AN1(II)=WET(II)*(DKK**2.*U2*DEXP(E3)*(BB)**2.*AJ1*VV1-DKK**2.
     & *DEXP(E3)*(BB)**2.*PAJ1*U3*VV1)*DEXP(DKK)
      AN2(II)=WET(II)*(-1.*DKK**2.*RAD(1)*U3*DEXP(E3)*(BB)**2.*VV1*AJ1
     & -DKK**2.*RAD(1)*U2*DEXP(E3)*(-BB)**2.*VV1*PAJ1)*DEXP(DKK)
2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN(IJ)
      SM2=SM2+AN1(IJ)
      SM3=SM3+AN2(IJ)
1999  CONTINUE
      RETURN
      END
```

Appendix E3-2: Computer programming source code for estimating the thermocapillary velocity of one spherical drop parallel two insulated plates.

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(500,501),RAD(2),DDK(96),WET(96),B(500,501),BF(500,3)
      INTEGER T,GG,LL1,LL2,LBB,LCC,GGG
      OPEN (24,FILE='WET3.DAT',STATUS='OLD')
      OPEN (25,FILE='DDTTH1-10-10.DAT',STATUS='NEW')
      OPEN (23,FILE='GAUSS80.DAT',STATUS='OLD')
      IN=80
      TR=1.D0
      BB=.1D0
      ETK=10.D0
      STA=10.D0
      CC=BB*TR
      DO 1001 I=1,IN
      READ (23,*) DDK(I),WET(I)
1001  CONTINUE
      T=1
      PI=DACOS(-1.D0)
      FI=0.01*PI/180.
      U4=DCOS(FI)
      U5=DSIN(FI)
      DO 3231    IUY=1,50
      READ (24,*) CV,NX
      RAD(1)=CV*BB
      GGG=2*NX
      DO 511 I=1,T
      DO 512 J=1,NX
      NU=J+NX*(I-1)
      NY=J+NX*(I-1)+T*NX
      DO 513 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      B(NU,GGG+1)=-1.*RAD(1)*U3*U4
      B(NY,GGG+1)=-1.*U3*U4
      DO 514 N=1,NX
      NZ=(2*N-1)+2*NX*(K-1)
      NL=2*N+2*NX*(K-1)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      B(NU,NZ)=R2**(-N-1)*W1*U4+SM1*U4
      B(NU,NL)=-R2**N*W1*U4
      B(NY,NZ)=(-N-1)*R2**(-N-2)*W1*U4+SM2
      B(NY,NL)=-ETK*N*R2**(N-1)*W1*U4
514   CONTINUE
513   CONTINUE
512   CONTINUE
511   CONTINUE
      LL1=500
      LL2=501
      LBB=GGG
      LCC=GGG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,B)
```

```
  GG=T*NX
  DO 7765 NN=1,2
  DO 111 I=1,T
  DO 112 J=1,NX
  NO=J+NX*(I-1)
  NP=J+NX*(I-1)+T*NX
  NQ=J+NX*(I-1)+2*T*NX
  NR=J+NX*(I-1)+3*T*NX
  NS=J+NX*(I-1)+4*T*NX
  NT=J+NX*(I-1)+5*T*NX
  DO 113 K=1,T
  CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
  IF (NN .EQ. 1) THEN
  A(NO,6*GG+1)=U3*U4
  A(NP,6*GG+1)=0.D0
  A(NQ,6*GG+1)=0.D0
  A(NR,6*GG+1)=0.D0
  A(NS,6*GG+1)=0.D0
  A(NT,6*GG+1)=0.D0
  END IF
  DO 114 N=1,NX
  NE=(6*N-5)+6*NX*(K-1)
  NF=(6*N-4)+6*NX*(K-1)
  NG=(6*N-3)+6*NX*(K-1)
  NH=(6*N-2)+6*NX*(K-1)
  NI=(6*N-1)+6*NX*(K-1)
  NJ=(6*N-0)+6*NX*(K-1)
  CALL FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
  CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
  CALL FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
  CALL XXD(FI,N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,
&WET,SUM1,SUM2,SUM3,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9,SUM10,
&SUM11,SUM12,SUM13,SUM14,SUM17,SUM18,SUM19,SUM20,SUM21,
&SUM22,SUM23,SUM24,SUM25,SUM26,SUM27,SUM28,SUM29,SUM30,
&SUM31,SUM32,SUM33,SUM34,SUM35,SUM36,SUM15,SUM16)

  AA1=((2.*N*(2*N-1)*U3*W1*U4**2.+(N-2)*WW2*DCOS(2.*FI)-N*(N+1)
&*(N-2)*WW)/2./R2**(N))
  BB1=-1.*(WWW2*DCOS(2.*FI)-N*(N+1)*WWW)/2./R2**(N+2)
  CC1=(W2*DCOS(2.*FI)+N*(N+1)*W)/2./R2**(N+1)
  AA2=(N*(2*N-1)*U3*W1+(N-2)*WW2)*U4*U5/R2**(N)
  BB2=-1.*(WWW2*U4*U5)/R2**(N+2)
  CC2=(W2*U4*U5)/R2**(N+1)
  AA3=(N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U4/R2**N
  BB3=-1.*(N*WWW1*U4)/R2**(N+2)
  CC3=-1.*(W1*U4)/R2**(N+1)

  AA1R=-1.*N*AA1/R2
  BB1R=-1.*(N+2)*BB1/R2
  CC1R=-1.*(N+1)*CC1/R2
  AA2R=-1.*N*AA2/R2
  BB2R=-1.*(N+2)*BB2/R2
  CC2R=-1.*(N+1)*CC2/R2
  AA3R=-1.*N*AA3/R2
  BB3R=-1.*(N+2)*BB3/R2
  CC3R=-1.*(N+1)*CC3/R2

  AA1S=(2.*N*(2*N-1)*U2*W1*U4**2.-2.*N*(2*N-1)*U3**2.*PW1*U4**2.-
```

```
&(N-2)*U3*PWW2*DCOS(2.*FI)+N*(N+1)*(N-2)*U3*PWW)/2./R2**N
  BB1S=-1.*(-1.*U3*PWWW2*DCOS(2.*FI)+N*(N+1)*U3*PWWW)/2.
&/R2**(N+2)
  CC1S=(-1.*U3*PW2*DCOS(2.*FI)-U3*N*(N+1)*PW)/2./R2**(N+1)
  AA2S=(U2*N*(2*N-1)*W1-N*(2*N-1)*U3**2.*PW1-U3*(N-2)*PWW2)*U4*
&U5/R2**N
  BB2S=(U3*PWWW2*U4*U5)/R2**(N+2)
  CC2S=(-1.*U3*PW2*U4*U5)/R2**(N+1)
  AA3S=(-1.*N*(2.*N-1)*U3*W1-U2*U3*N*(2*N-1)*PW1+U3*(N+1)*(N-2)
&*PWW1)*U4/R2**N
  BB3S=U3*N*PWWW1*U4/R2**(N+2)
  CC3S=U3*PW1*U4/R2**(N+1)
  AA1F=((-2.*N*(2*N-1)*U3*W1*U4*U5-(N-2)*WW2*DSIN(2.*FI))
&/R2**(N))
  BB1F=WWW2*DSIN(2.*FI)/R2**(N+2)
  CC1F=-1.*W2*DSIN(2.*FI)/R2**(N+1)
  AA2F=(N*(2*N-1)*U3*W1+(N-2)*WW2)*DCOS(2.*FI)/R2**(N)
  BB2F=-1.*(WWW2*DCOS(2.*FI))/R2**(N+2)
  CC2F=(W2*DCOS(2.*FI))/R2**(N+1)
  AA3F=-1.*(N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U5/R2**N
  BB3F=(N*WWW1*U5)/R2**(N+2)
  CC3F=(W1*U5)/R2**(N+1)

  A(NO,NE)=U3*U4*(AA1+SUM1)+U3*U5*(AA2+SUM2)+U2*(AA3+SUM3)
  A(NO,NG)=U3*U4*(BB1+SUM4)+U3*U5*(BB2+SUM5)+U2*(BB3+SUM6)
  A(NO,NI)=U3*U4*(CC1+SUM7)+U3*U5*(CC2+SUM8)+U2*(CC3+SUM9)
  A(NO,NF)=0.D0
  A(NO,NH)=0.D0
  A(NO,NJ)=0.D0
  A(NP,NE)=U3*U4*(AA1+SUM1)+U3*U5*(AA2+SUM2)+U2*(AA3+SUM3)
  A(NP,NG)=U3*U4*(BB1+SUM4)+U3*U5*(BB2+SUM5)+U2*(BB3+SUM6)
  A(NP,NI)=U3*U4*(CC1+SUM7)+U3*U5*(CC2+SUM8)+U2*(CC3+SUM9)
  A(NP,NF)=0.D0
  A(NP,NH)=-N*R2**(N-1)*W1*U4
  A(NP,NJ)=-N*R2**(N+1)*W1*U4/2./STA/(2*N+3)
  A(NQ,NE)=U2*U4*(AA1+SUM1)+U2*U5*(AA2+SUM2)-U3*(AA3+SUM3)
  A(NQ,NG)=U2*U4*(BB1+SUM4)+U2*U5*(BB2+SUM5)-U3*(BB3+SUM6)
  A(NQ,NI)=U2*U4*(CC1+SUM7)+U2*U5*(CC2+SUM8)-U3*(CC3+SUM9)
  A(NQ,NF)=-1.*R2**N*W1*U4/U3
  A(NQ,NH)=R2**(N-1)*PW1*U3*U4
  A(NQ,NJ)=(N+3)*R2**(N+1)*PW1*U4*U3/2./STA/(2*N+3)/(N+1)
  A(NR,NE)=-1.*U5*(AA1+SUM1)+U4*(AA2+SUM2)
  A(NR,NG)=-1.*U5*(BB1+SUM4)+U4*(BB2+SUM5)
  A(NR,NI)=-1.*U5*(CC1+SUM7)+U4*(CC2+SUM8)
  A(NR,NF)=-1.*R2**N*PW1*U3*U5
  A(NR,NH)=R2**(N-1)*W1*U5/U3
  A(NR,NJ)=(N+3)*R2**(N+1)*W1*U5/U3/2./STA/(2*N+3)/(N+1)
  A(NS,NE)=U2*U4*(AA1R+SUM10)+U2*U5*(AA2R+SUM11)-
&U3*(AA3R+SUM12)+(U3*U4*(AA1S+SUM19)+U3*U5*(AA2S+SUM20)
&+U2*(AA3S+SUM21))/R2
  A(NS,NG)=U2*U4*(BB1R+SUM13)+U2*U5*(BB2R+SUM14)-
&U3*(BB3R+SUM15)+(U3*U4*(BB1S+SUM22)+U3*U5*(BB2S+SUM23)
&+U2*(BB3S+SUM24))/R2
  A(NS,NI)=U2*U4*(CC1R+SUM16)+U2*U5*(CC2R+SUM17)-
&U3*(CC3R+SUM18)+(U3*U4*(CC1S+SUM25)+U3*U5*(CC2S+SUM26)
&+U2*(CC3S+SUM27))/R2
  A(NS,NF)=-1.*STA*(N-1)*R2**(N-1)*W1*U4/U3
  A(NS,NH)=2.*STA*(N-1)*R2**(N-2)*U3*U4*PW1
```

```
      A(NS,NJ)=N*(N+2)*R2**N*U3*U4*PW1/(N+1)/(2*N+3)
      A(NT,NE)=-1.*U5*(AA1R+SUM10)+U4*(AA2R+SUM11)
     &+(U4*(AA1F+SUM28)+U5*(AA2F+SUM29)+U2*(AA3F+SUM30)/U3)/R2
      A(NT,NG)=-1.*U5*(BB1R+SUM13)+U4*(BB2R+SUM14)
     &+(U4*(BB1F+SUM31)+U5*(BB2F+SUM32)+U2*(BB3F+SUM33)/U3)/R2
      A(NT,NI)=-1.*U5*(CC1R+SUM16)+U4*(CC2R+SUM17)
     &+(U4*(CC1F+SUM34)+U5*(CC2F+SUM35)+U2*(CC3F+SUM36)/U3)/R2
      A(NT,NF)=-1.*STA*(N-1)*R2**(N-1)*PW1*U5*U3
      A(NT,NH)=2.*STA*(N-1)*R2**(N-2)*U5*W1/U3
      A(NT,NJ)=N*(N+2)*R2**N*U5*W1/U3/(N+1)/(2*N+3)
114   CONTINUE
113   CONTINUE
112   CONTINUE
111   CONTINUE
      IF (NN .EQ. 2) THEN
      DO 811 J=1,NX
      NO=J
      NP=J+NX
      NQ=J+2*NX
      NR=J+3*NX
      NS=J+4*NX
      NT=J+5*NX
      CALL FU(1,J,1,NX,RAD,PI,U2,U3,R2)
      VALUE=0.D0
      VALUE1=0.D0
      DO 713 KK=1,NX
      NZ=2*KK-1
      CALL FUCK2(U2,KK,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL XRD(KK,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      VALUE=VALUE+B(NZ,GGG+1)*(R2**(-KK-1)*PW1*U4*(-1.*U3)+SM3)
      VALUE1=VALUE1+B(NZ,GGG+1)*(R2**(-KK-1)*W1*(-1.*U5)-U5*SM1)
713   CONTINUE
      A(NO,6*GG+1)=0.D0
      A(NP,6*GG+1)=0.D0
      A(NQ,6*GG+1)=0.D0
      A(NR,6*GG+1)=0.D0
      A(NS,6*GG+1)=(RAD(1)*U2*U4+VALUE)/RAD(1)
      A(NT,6*GG+1)=(-1.*RAD(1)*U3*U5+VALUE1)/RAD(1)/U3
811   CONTINUE
      END IF
      LL1=500
      LL2=501
      LBB=6*GG
      LCC=6*GG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,A)
      DO 999 I=1,6*GG
      BF(I,NN)=A(I,6*GG+1)
999   CONTINUE
7765  CONTINUE
      VVU=2.*RAD(1)/(2.+3.*STA)/(2.+ETK)
      HGD=-1.*BF(1,2)/BF(1,1)/VVU
      WRITE (*,9) CV,HGD
      WRITE (25,9) CV,HGD
3231  CONTINUE
9     FORMAT (2(F12.5))
      STOP
      END
```

```fortran
      SUBROUTINE FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION RAD(2)
      PID=1.D-3
      DTHETA=(PI-4.D0*PID)/(NX-2)
      IF(J==1) THEN
      Z=RAD(I)*DCOS(PID)
      V=RAD(I)*DSIN(PID)
      END IF
      IF((1<J) .AND. (J<=NX/2)) THEN
      Z=RAD(I)*DCOS(PID+(J-1)*DTHETA)
      V=RAD(I)*DSIN(PID+(J-1)*DTHETA)
      END IF
      IF(NX/2<J) THEN
      Z=RAD(I)*DCOS(PI/2.D0+(J-1-NX/2)*DTHETA)
      V=RAD(I)*DSIN(PI/2.D0+(J-1-NX/2)*DTHETA)
      END IF
      U2=Z/RAD(I)
      U3=V/RAD(I)
      R2=RAD(I)
      RETURN
      END

      SUBROUTINE GAUSL (N,M,II,JJ,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(N,M)
      DO 10 I=1,II
      AA=0.E0
      DO 9 J=1,II
9     AA=AA+ABS(A(I,J))
      DO 10 J=1,JJ
10    A(I,J)=A(I,J)/AA
      CALL XXXXX (N,M,II,JJ-II,A)
      RETURN
      END

      SUBROUTINE XXXXX (ND,NCOL,N,NS,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(ND,NCOL)
      N1=N+1
      NT=N+NS
      IF(N.EQ.1) GO TO 50
      DO 10 I=2,N
      IP=I-1
      I1=IP
      X=ABS(A(I1,I1))
      DO 11 J=I,N
      IF(ABS(A(J,I1)).LT.X) GO TO 11
      X=ABS(A(J,I1))
      IP=J
11    CONTINUE
      IF(IP.EQ.I1) GO TO 13
      DO 12 J=I1,NT
      X=A(I1,J)
      A(I1,J)=A(IP,J)
12    A(IP,J)=X
13    DO 10 J=I,N
      X=A(J,I1)/A(I1,I1)
```

```
      DO 10 K=I,NT
10    A(J,K)=A(J,K)-X*A(I1,K)
50    DO 20 IP=1,N
      I=N1-IP
      DO 20 K=N1,NT
      A(I,K)=A(I,K)/A(I,I)
      IF(I.EQ.1) GO TO 20
      I1=I-1
      DO 25 J=1,I1
25    A(J,K)=A(J,K)-A(I,K)*A(J,I)
20    CONTINUE
      RETURN
      END

      SUBROUTINE FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PA(-1:600)
      PA(-1)=0.D0
      PA(0)=0.D0
      PA(1)=(1.-U2**2)**.5
      PA(2)=3.*U2*(1.-U2**2)**.5
      DO 100 J=1,N+1
      PA(J+1)=((2*J+1)*U2*PA(J)-(J+1)*PA(J-1))/(J)
100   CONTINUE
      W1=PA(N)
      WW1=PA(N-1)
      WWW1=PA(N+1)
      PW1=(N*U2*PA(N)-(N+1)*PA(N-1))/(U2**2.-1.)
      PWW1=((N-1)*U2*PA(N-1)-(N)*PA(N-2))/(U2**2.-1.)
      PWWW1=((N+1)*U2*PA(N+1)-(N+2)*PA(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PR(-1:600)
      PR(-1)=0.D0
      PR(0)=1.D0
      PR(1)=U2
      DO 34 I=2,N+1
      PR(I)=((2*I-1)*U2*PR(I-1)-(I-1)*PR(I-2))/I
34    CONTINUE
      W=PR(N)
      WW=PR(N-1)
      WWW=PR(N+1)
      PW=(N*U2*PR(N)-N*PR(N-1))/(U2**2.-1.)
      PWW=((N-1)*U2*PR(N-1)-(N-1)*PR(N-2))/(U2**2.-1.)
      PWWW=((N+1)*U2*PR(N+1)-(N+1)*PR(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PB(-1:600)
      PB(-1)=0.D0
      PB(0)=0.D0
      PB(1)=0.D0
      PB(2)=3.*(1.-U2**2)
```

```
      DO 150 K=2,N+1
      PB(K+1)=((2*K+1)*U2*PB(K)-(K+2)*PB(K-1))/(K-1)
150   CONTINUE
      W2=PB(N)
      WW2=PB(N-1)
      WWW2=PB(N+1)
      PW2=(N*U2*PB(N)-(N+2)*PB(N-1))/(U2**2.-1.)
      PWW2=((N-1)*U2*PB(N-1)-(N+1)*PB(N-2))/(U2**2.-1.)
      PWWW2=((N+1)*U2*PB(N+1)-(N+3)*PB(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE XXD(FI,N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,
     &SUM1,SUM2,SUM3,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9,SUM10,
     &SUM11,SUM12,SUM13,SUM14,SUM17,SUM18,SUM19,SUM20,SUM21,
     &SUM22,SUM23,SUM24,SUM25,SUM26,SUM27,SUM28,SUM29,SUM30,
     &SUM31,SUM32,SUM33,SUM34,SUM35,SUM36,SUM15,SUM16)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),RAD(2)
      DIMENSION ANN1(96),ANN2(96),ANN3(96),BNN1(96),
     &BNN2(96),BNN3(96)
      DIMENSION CNN1(96),CNN2(96),CNN3(96),ANN1R(96),
     &ANN2R(96),ANN3R(96)
      DIMENSION BNN1R(96),BNN2R(96),BNN3R(96),CNN1R(96),CNN2R(96)
      DIMENSION CNN3R(96),ANN1S(96),ANN2S(96),ANN3S(96),BNN1S(96)
      DIMENSION BNN2S(96),BNN3S(96),CNN1S(96),CNN2S(96),CNN3S(96)
      DIMENSION ANN1F(96),ANN2F(96),ANN3F(96),BNN1F(96),BNN2F(96)
      DIMENSION BNN3F(96),CNN1F(96),CNN2F(96),CNN3F(96)
      DO 2001 II=1,IN
      Z=RAD(1)*U2
      X=RAD(1)*U3*U4
      Y=RAD(1)*U3*U5
      DKK=DDK(II)
      DY=RAD(1)*U3
      DDY=DKK*DY
      CALL BESSEL(DDY,AJ,AJ0,AJ1,AJ2)
      PAJ0=-1.*AJ1
      PAJ1=.5*(AJ0-AJ2)
      B1=AJ0*X**2.+(Y**2.-X**2.)*AJ1/DDY
      B2=(AJ0-2.*AJ1/DDY)/DDY**2.
      B1R=(X**2.*PAJ0*DDY+2.*X**2.*AJ0+(Y**2.-X**2.)*(AJ1+PAJ1*DDY)
     &/DDY)/RAD(1)
      B1S=Z*(X**2.*PAJ0*DDY+2.*X**2.*AJ0+(Y**2.-X**2.)*(AJ1+PAJ1*DDY
     &)/DDY)/DY
      B1F=-2.*X*Y*AJ0+4*X*Y*AJ1/DDY
      B2R=(6.*AJ1/DDY-2.*AJ0+DDY*PAJ0-2.*PAJ1)/RAD(1)/DDY**2.
      B2S=Z*(6.*AJ1/DDY-2.*AJ0+DDY*PAJ0-2.*PAJ1)/DDY**2./DY
      E3=DKK*(Z+BB)
      E2=DKK*(Z-CC)
      E1=DKK*(BB+CC)
      DEL1=2.*DSINH(E1)
      DEL2=4.*((DSINH(E1))**2.-E1**2.)
      G1=4.*E1*E2*E3*(DSINH(E3)/E3+DSINH(E1)*DSINH(E2)/E1/E2)/DEL2
      G2=4.*E1*E2*E3*(DSINH(E3)/E3-DSINH(E1)*DSINH(E2)/E1/E2)/DEL2
      D1=4.*E1*E3*E2*(DSINH(E2)/E2+DSINH(E1)*DSINH(E3)/E1/E3)/DEL2
      D2=4.*E1*E3*E2*(DSINH(E2)/E2-DSINH(E1)*DSINH(E3)/E1/E3)/DEL2
      G1R=4*E1*DKK*U2*(E2+E3)*(DSINH(E3)/E3+DSINH(E1)*DSINH(E2)
     &/E2/E1)
```

```
&/DEL2+4.*E1*E2*E3*DKK*U2*(DCOSH(E3)/E3-DSINH(E3)/E3**2.+
&DSINH(E1)*DCOSH(E2)/E2/E1-DSINH(E1)*DSINH(E2)/E1/E2**2.)/DEL2
  G2R=4*E1*DKK*U2*(E2+E3)*(DSINH(E3)/E3-
&DSINH(E1)*DSINH(E2)/E2/E1)
&/DEL2+4.*E1*E2*E3*DKK*U2*(DCOSH(E3)/E3-DSINH(E3)/E3**2.-
&DSINH(E1)*DCOSH(E2)/E2/E1+DSINH(E1)*DSINH(E2)/E1/E2**2.)/DEL2
  D1R=4*E1*DKK*U2*(E2+E3)*(DSINH(E2)/E2+DSINH(E1)*DSINH(E3)
&/E3/E1)/DEL2+4.*E1*E2*E3*DKK*U2*(DCOSH(E2)/E2-DSINH(E2)/E2**2.+
& DSINH(E1)*DCOSH(E3)/E3/E1-DSINH(E1)*DSINH(E3)/E1/E3**2.)/DEL2
  D2R=4*E1*DKK*U2*(E2+E3)*(DSINH(E2)/E2-DSINH(E1)*DSINH(E3)
&/E3/E1)
&/DEL2+4.*E1*E2*E3*DKK*U2*(DCOSH(E2)/E2-DSINH(E2)/E2**2.-
&DSINH(E1)*DCOSH(E3)/E3/E1+DSINH(E1)*DSINH(E3)/E1/E3**2.)/DEL2
  G1S=-1.*RAD(1)*U3*G1R/U2
  G2S=-1.*RAD(1)*U3*G2R/U2
  D1S=-1.*RAD(1)*U3*D1R/U2
  D2S=-1.*RAD(1)*U3*D2R/U2
  G3=4.*E1*(E2*(DCOSH(E3)-DSINH(E1)*DSINH(E2)/E1/E2)
&+E3*(DSINH(E3)/E3-DSINH(E1)*DCOSH(E2)/E1))/DEL2
  G4=4.*E1*(E2*(DCOSH(E3)-DSINH(E1)*DSINH(E2)/E1/E2)
&-E3*(DSINH(E3)/E3-DSINH(E1)*DCOSH(E2)/E1))/DEL2
  D3=4.*E1*(E3*(DCOSH(E2)-DSINH(E1)*DSINH(E3)/E1/E3)
&+E2*(DSINH(E2)/E2-DSINH(E1)*DCOSH(E3)/E1))/DEL2
  D4=4.*E1*(E3*(DCOSH(E2)-DSINH(E1)*DSINH(E3)/E1/E3)
&-E2*(DSINH(E2)/E2-DSINH(E1)*DCOSH(E3)/E1))/DEL2
  G3R=4.*E1*DKK*U2*((DCOSH(E3)-DSINH(E1)*DSINH(E2)/E1/E2)
&+E2*(DSINH(E3)-DSINH(E1)*DCOSH(E2)/E1/E2
&+DSINH(E1)*DSINH(E2)/E1/E2**2.)+(DSINH(E3)/E3-
&DSINH(E1)*DCOSH(E2)/E1)+E3*(DCOSH(E3)/E3-DSINH(E3)/
&E3**2.-DSINH(E1)*DSINH(E2)/E1))/DEL2
  G4R=4.*E1*DKK*U2*((DCOSH(E3)-DSINH(E1)*DSINH(E2)/E1/E2)
&+E2*(DSINH(E3)-DSINH(E1)*DCOSH(E2)/E1/E2
&+DSINH(E1)*DSINH(E2)/E1/E2**2.)-(DSINH(E3)/E3-
&DSINH(E1)*DCOSH(E2)/E1)-E3*(DCOSH(E3)/E3-DSINH(E3)/
&E3**2.-DSINH(E1)*DSINH(E2)/E1))/DEL2
  D3R=4.*E1*DKK*U2*((DCOSH(E2)-
&DSINH(E1)*DSINH(E3)/E1/E3)+E3*(DSINH
&(E2)-DSINH(E1)*DCOSH(E3)/E1/E3+DSINH(E1)*DSINH(E3)/E1/E3**2.)+(
&DSINH(E2)/E2-DSINH(E1)*DCOSH(E3)/E1)+E2*(DCOSH(E2)/E2-
&DSINH(E2)/E2**2.-DSINH(E1)*DSINH(E3)/E1))/DEL2
  D4R=4.*E1*DKK*U2*((DCOSH(E2)-
&DSINH(E1)*DSINH(E3)/E1/E3)+E3*(DSINH
&(E2)-DSINH(E1)*DCOSH(E3)/E1/E3+DSINH(E1)*DSINH(E3)/E1/E3**2.)-(
&DSINH(E2)/E2-DSINH(E1)*DCOSH(E3)/E1)-E2*(DCOSH(E2)/E2-
&DSINH(E2)/E2**2.-DSINH(E1)*DSINH(E3)/E1))/DEL2
  G3S=-1.*RAD(1)*U3*G3R/U2
  G4S=-1.*RAD(1)*U3*G4R/U2
  D3S=-1.*RAD(1)*U3*D3R/U2
  D4S=-1.*RAD(1)*U3*D4R/U2
  G5=-2.*DSINH(E2)/DEL1
  G5R=-2.*DKK*U2*DCOSH(E2)/DEL1
  G5S=2.*RAD(1)*DKK*U3*DCOSH(E2)/DEL1
  D5=-2.*DSINH(E3)/DEL1
  D5R=-2.*DKK*U2*DCOSH(E3)/DEL1
  D5S=2.*RAD(1)*DKK*U3*DCOSH(E3)/DEL1
  G6=8.*E1**2.*(E3*DSINH(E1)*(DSINH(E3)/E3-
&DSINH(E1)*DCOSH(E2)/E1)/
& E1+E2*(DSINH(E1)*DCOSH(E3)/E1-DSINH(E2)/E2))/DEL1/DEL2
```

```
  D6=8.*E1**2.*(E2*DSINH(E1)*(DSINH(E2)/E2-
&DSINH(E1)*DCOSH(E3)/E1)/
&E1+E3*(DSINH(E1)*DCOSH(E2)/E1-DSINH(E3)/E3))/DEL1/DEL2
  G6R=8.*E1**2.*DKK*U2*(DSINH(E1)*(DSINH(E3)/E3-
&DSINH(E1)*DCOSH(E2)
&/E1)/E1+E3*DSINH(E1)*(DCOSH(E3)/E3-DSINH(E3)/E3**2.-DSINH(E1)*
&DSINH(E2)/E1)/E1+(DSINH(E1)*DCOSH(E3)/E1-
&DSINH(E2)/E2)+E2*(DSINH(
&E1)*DSINH(E3)/E1-DCOSH(E2)/E2+DSINH(E2)/E2**2.))/DEL1/DEL2
  D6R=8.*E1**2.*DKK*U2*(DSINH(E1)*(DSINH(E2)/E2-
&DSINH(E1)*DCOSH(E3)
&/E1)/E1+E2*DSINH(E1)*(DCOSH(E2)/E2-DSINH(E2)/E2**2.-DSINH(E1)*
&DSINH(E3)/E1)/E1+(DSINH(E1)*DCOSH(E2)/E1-
&DSINH(E3)/E3)+E3*(DSINH(
&E1)*DSINH(E2)/E1-DCOSH(E3)/E3+DSINH(E3)/E3**2.))/DEL1/DEL2
  G6S=-1.*RAD(1)*U3*G6R/U2
  D6S=-1.*RAD(1)*U3*D6R/U2
  CALL BEST(N,1,1,0,DKK,-BB,F1)
  CALL BEST(N,1,2,1,DKK,-BB,F2)
  CALL BEST(N-1,2,2,3,DKK,-BB,F3)
  CALL BEST(N-1,0,0,1,DKK,-BB,F4)
  CALL BEST(N-1,2,2,1,DKK,-BB,F5)
  CALL BEST(N-1,1,1,0,DKK,-BB,F6)
  CALL BEST(N+1,2,2,3,DKK,-BB,F7)
  CALL BEST(N+1,0,0,1,DKK,-BB,F8)
  CALL BEST(N+1,2,2,1,DKK,-BB,F9)
  CALL BEST(N+1,1,1,0,DKK,-BB,F10)
  CALL BEST(N,2,2,3,DKK,-BB,F11)
  CALL BEST(N,0,0,1,DKK,-BB,F12)
  CALL BEST(N,2,2,1,DKK,-BB,F13)
  CALL BEST(N,1,1,2,DKK,-BB,F14)
  CALL BEST(N-1,0,0,3,DKK,-BB,F15)
  CALL BEST(N,1,2,3,DKK,-BB,F16)
  CALL BEST(N-1,1,1,2,DKK,-BB,F17)
  CALL BEST(N+1,0,0,3,DKK,-BB,F18)
  CALL BEST(N+1,1,1,2,DKK,-BB,F19)
  CALL BEST(N,0,0,3,DKK,-BB,F20)
  CALL BEST(N,1,1,0,DKK,CC,T1)
  CALL BEST(N,1,2,1,DKK,CC,T2)
  CALL BEST(N-1,2,2,3,DKK,CC,T3)
  CALL BEST(N-1,0,0,1,DKK,CC,T4)
  CALL BEST(N-1,2,2,1,DKK,CC,T5)
  CALL BEST(N-1,1,1,0,DKK,CC,T6)
  CALL BEST(N+1,2,2,3,DKK,CC,T7)
  CALL BEST(N+1,0,0,1,DKK,CC,T8)
  CALL BEST(N+1,2,2,1,DKK,CC,T9)
  CALL BEST(N+1,1,1,0,DKK,CC,T10)
  CALL BEST(N,2,2,3,DKK,CC,T11)
  CALL BEST(N,0,0,1,DKK,CC,T12)
  CALL BEST(N,2,2,1,DKK,CC,T13)
  CALL BEST(N,1,1,2,DKK,CC,T14)
  CALL BEST(N-1,0,0,3,DKK,CC,T15)
  CALL BEST(N,1,2,3,DKK,CC,T16)
  CALL BEST(N-1,1,1,2,DKK,CC,T17)
  CALL BEST(N+1,0,0,3,DKK,CC,T18)
  CALL BEST(N+1,1,1,2,DKK,CC,T19)
  CALL BEST(N,0,0,3,DKK,CC,T20)
  H1=-N*(2*N-1)*(-BB)**2.*AJ0*F1+N*(2*N-1)*(-BB)**2.*B1*F2/DY**2.-
```

```
&.5*(N-2)*(Y**2.-X**2.)*B2*F3+.5*N*(N+1)*(N-2)*AJ0*F4
  H1C=-N*(2*N-1)*CC**2.*AJ0*T1+N*(2*N-1)*CC**2.*B1*T2/DY**2.-
&.5*(N-2)*(Y**2.-X**2.)*B2*T3+.5*N*(N+1)*(N-2)*AJ0*T4
  H1R=-N*(2*N-1)*(-BB)**2.*PAJ0*DKK*U3*F1-2.*N*(2*N-1)*U3*(-BB)**2.
&*B1*F2/DY**3.+N*(2*N-1)*(-BB)**2.*B1R*F2/DY**2.-(N-2)*(Y**2.-
&X**2.)*B2*F3/RAD(1)-.5*(N-2)*(Y**2.-X**2.)*B2R*F3+.5*N*(N+1)*(N-
&2)*PAJ0*DKK*U3*F4
  H1CR=-N*(2*N-1)*CC**2.*PAJ0*DKK*U3*T1-2.*N*(2*N-1)*U3*CC**2.
&*B1*T2/DY**3.+N*(2*N-1)*CC**2.*B1R*T2/DY**2.-(N-2)*(Y**2.-
&X**2.)*B2*T3/RAD(1)-.5*(N-2)*(Y**2.-X**2.)*B2R*T3+.5*N*(N+1)*(N-
&2)*PAJ0*DKK*U3*T4
  H1S=-N*(2*N-1)*(-BB)**2.*PAJ0*DKK*RAD(1)*U2*F1-2.*N*(2*N-1)*U2*
&RAD(1)*(-BB)**2.*B1*F2/DY**3.+N*(2*N-1)*(-BB)**2.*B1S*F2/DY**2.
&-(N-2)*(Y**2.-X**2.)*B2*F3*Z/DY-.5*(N-2)*(Y**2.-X**2.)*B2S*F3
&+.5*N*(N+1)*(N-2)*DKK*RAD(1)*U2*F4*PAJ0
  H1CS=-N*(2*N-1)*CC**2.*PAJ0*DKK*RAD(1)*U2*T1-2.*N*(2*N-1)*U2*
&RAD(1)*CC**2.*B1*T2/DY**3.+N*(2*N-1)*CC**2.*B1S*T2/DY**2.
&-(N-2)*(Y**2.-X**2.)*B2*T3*Z/DY-.5*(N-2)*(Y**2.-X**2.)*B2S*T3
&+.5*N*(N+1)*(N-2)*DKK*RAD(1)*U2*T4*PAJ0
  H1F=N*(2*N-1)*(-BB)**2.*B1F*F2/DY**2.-2.*(N-2)*X*Y*B2*F3
  H1CF=N*(2*N-1)*CC**2.*B1F*T2/DY**2.-2.*(N-2)*X*Y*B2*T3
  H2=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
&(N+1)*(N-2)*F4)*B1/DY**2.
  H2C=(-1.*N*(2*N-1)*CC**2.*(T1-T2)+.5*(N-2)*CC**2.*T5+.5*N*
&(N+1)*(N-2)*T4)*B1/DY**2.
  H2R=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
&(N+1)*(N-2)*F4)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H2CR=(-1.*N*(2*N-1)*CC**2.*(T1-T2)+.5*(N-2)*CC**2.*T5+.5*N*
&(N+1)*(N-2)*T4)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H2S=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
&(N+1)*(N-2)*F4)*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H2CS=(-1.*N*(2*N-1)*CC**2.*(T1-T2)+.5*(N-2)*CC**2.*T5+.5*N*
&(N+1)*(N-2)*T4)*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H2F=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
&(N+1)*(N-2)*F4)*B1F/DY**2.
  H2CF=(-1.*N*(2*N-1)*CC**2.*(T1-T2)+.5*(N-2)*CC**2.*T5+.5*N*
&(N+1)*(N-2)*T4)*B1F/DY**2.
  H3=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*B1/DY**2.
  H3C=DKK*CC**2.*(-1.*N*(2*N-1)*CC*T1+(N+1)*(N-2)*T6)*B1/DY**2.
  H3R=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*(B1R/
&DY**2.-2.*U3*B1/DY**3.)
  H3CR=DKK*CC**2.*(-1.*N*(2*N-1)*CC*T1+(N+1)*(N-2)*T6)*(B1R/
&DY**2.-2.*U3*B1/DY**3.)
  H3S=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*(B1S/
&DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H3CS=DKK*CC**2.*(-1.*N*(2*N-1)*CC*T1+(N+1)*(N-2)*T6)*(B1S/
&DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H3F=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*B1F/
&DY**2.
  H3CF=DKK*CC**2.*(-1.*N*(2*N-1)*CC*T1+(N+1)*(N-2)*T6)*B1F/
&DY**2.
  H4=.5*((Y**2.-X**2.)*B2*F7-N*(N+1)*AJ0*F8)
  H4C=.5*((Y**2.-X**2.)*B2*T7-N*(N+1)*AJ0*T8)
  H4R=.5*(2.*(Y**2.-X**2.)*B2*F7/RAD(1)+(Y**2.-X**2.)*B2R*F7-N*
&(N+1)*PAJ0*DKK*U3*F8)
  H4CR=.5*(2.*(Y**2.-X**2.)*B2*T7/RAD(1)+(Y**2.-X**2.)*B2R*T7-N*
&(N+1)*PAJ0*DKK*U3*T8)
  H4S=.5*(2.*Z*(Y**2.-X**2.)*B2*F7/DY+(Y**2.-X**2.)*B2S*F7-N*(N+1)
```

```
&*PAJ0*DKK*RAD(1)*U2*F8)
  H4CS=.5*(2.*Z*(Y**2.-X**2.)*B2*T7/DY+(Y**2.-X**2.)*B2S*T7-N*(N+1)
&*PAJ0*DKK*RAD(1)*U2*T8)
  H4F=2.*X*Y*B2*F7
  H4CF=2.*X*Y*B2*T7
  H5=-.5*((-BB)**2.*F9+N*(N+1)*F8)*B1/DY**2.
  H5C=-.5*(CC**2.*T9+N*(N+1)*T8)*B1/DY**2.
  H5R=-.5*((-BB)**2.*F9+N*(N+1)*F8)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H5CR=-.5*(CC**2.*T9+N*(N+1)*T8)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H5S=-.5*((-BB)**2.*F9+N*(N+1)*F8)*(B1S/DY**2.-2.*RAD(1)*U2*B1/
&DY**3.)
  H5CS=-.5*(CC**2.*T9+N*(N+1)*T8)*(B1S/DY**2.-2.*RAD(1)*U2*B1/
&DY**3.)
  H5F=-.5*((-BB)**2.*F9+N*(N+1)*F8)*B1F/DY**2.
  H5CF=-.5*(CC**2.*T9+N*(N+1)*T8)*B1F/DY**2.
  H6=N*DKK*(-BB)**2.*B1*F10/DY**2.
  H6R=N*DKK*(-BB)**2.*F10*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H6S=N*DKK*(-BB)**2.*F10*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H6F=N*DKK*(-BB)**2.*F10*B1F/DY**2.
  H6C=N*DKK*CC**2.*B1*T10/DY**2.
  H6CR=N*DKK*CC**2.*T10*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H6CS=N*DKK*CC**2.*T10*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H6CF=N*DKK*CC**2.*T10*B1F/DY**2.
  H7=-.5*((Y**2.-X**2.)*B2*F11+N*(N+1)*AJ0*F12)
  H7R=-.5*(2.*(Y**2.-X**2.)*B2*F11/RAD(1)+(Y**2.-X**2.)*B2R*F11+N*
&(N+1)*PAJ0*DKK*U3*F12)
  H7S=-.5*(2.*(Y**2.-X**2.)*Z*B2*F11/DY+(Y**2.-X**2.)*B2S*F11+N*
&(N+1)*PAJ0*DKK*U2*RAD(1)*F12)
  H7F=-2.*X*Y*B2*F11
  H7C=-.5*((Y**2.-X**2.)*B2*T11+N*(N+1)*AJ0*T12)
  H7CR=-.5*(2.*(Y**2.-X**2.)*B2*T11/RAD(1)+(Y**2.-X**2.)*B2R*T11+N*
&(N+1)*PAJ0*DKK*U3*T12)
  H7CS=-.5*(2.*(Y**2.-X**2.)*Z*B2*T11/DY+(Y**2.-X**2.)*B2S*T11+N*
&(N+1)*PAJ0*DKK*U2*RAD(1)*T12)
  H7CF=-2.*X*Y*B2*T11
  H8=.5*((-BB)**2.*F13-N*(N+1)*F12)*B1/DY**2.
  H8R=.5*((-BB)**2.*F13-N*(N+1)*F12)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H8S=.5*((-BB)**2.*F13-N*(N+1)*F12)*(B1S/DY**2.-2.*U2*RAD(1)*B1/
&DY**3.)
  H8F=.5*((-BB)**2.*F13-N*(N+1)*F12)*B1F/DY**2.
  H8C=.5*(CC**2.*T13-N*(N+1)*T12)*B1/DY**2.
  H8CR=.5*(CC**2.*T13-N*(N+1)*T12)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H8CS=.5*(CC**2.*T13-N*(N+1)*T12)*(B1S/DY**2.-2.*U2*RAD(1)*B1/
&DY**3.)
  H8CF=.5*(CC**2.*T13-N*(N+1)*T12)*B1F/DY**2.
  H9=DKK*(-BB)**2.*F1*B1/DY**2.
  H9R=DKK*(-BB)**2.*F1*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H9S=DKK*(-BB)**2.*F1*(B1S/DY**2.-2.*U2*RAD(1)*B1/DY**3.)
  H9F=DKK*(-BB)**2.*F1*B1F/DY**2.
  H9C=DKK*CC**2.*T1*B1/DY**2.
  H9CR=DKK*CC**2.*T1*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H9CS=DKK*CC**2.*T1*(B1S/DY**2.-2.*U2*RAD(1)*B1/DY**3.)
  H9CF=DKK*CC**2.*T1*B1F/DY**2.
  H10=X*Y*B2*(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15
&/(-BB)**2.)
  H10R=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
&**2.)*(2.*X*Y*B2/RAD(1)+X*Y*B2R)
  H10S=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
```

```
&**2.)*(2.*Z*X*Y*B2/DY+X*Y*B2S)
  H10F=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
&**2.)*DY**2.*B2*DCOS(2.*FI)
  H10C=X*Y*B2*(-1.*N*(2*N-1)*T14-.5*(N-2)*T3+.5*N*(N+1)*(N-2)*T15
&/CC**2.)
  H10CR=(-1.*N*(2*N-1)*T14-.5*(N-2)*T3+.5*N*(N+1)*(N-2)*T15/CC
&**2.)*(2.*X*Y*B2/RAD(1)+X*Y*B2R)
  H10CS=(-1.*N*(2*N-1)*T14-.5*(N-2)*T3+.5*N*(N+1)*(N-2)*T15/CC
&**2.)*(2.*Z*X*Y*B2/DY+X*Y*B2S)
  H10CF=(-1.*N*(2*N-1)*T14-.5*(N-2)*T3+.5*N*(N+1)*(N-2)*T15/CC
&**2.)*DY**2.*B2*DCOS(2.*FI)
  H11=X*Y*B2*(N*(2*N-1)*F16+(N-2)*F3)
  H11R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(N*(2*N-1)*F16+(N-2)*F3)
  H11S=(2.*Z*X*Y*B2/DY+X*Y*B2S)*(N*(2*N-1)*F16+(N-2)*F3)
  H11F=DY**2.*B2*DCOS(2.*FI)*(N*(2*N-1)*F16+(N-2)*F3)
  H11C=X*Y*B2*(N*(2*N-1)*T16+(N-2)*T3)
  H11CR=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(N*(2*N-1)*T16+(N-2)*T3)
  H11CS=(2.*Z*X*Y*B2/DY+X*Y*B2S)*(N*(2*N-1)*T16+(N-2)*T3)
  H11CF=DY**2.*B2*DCOS(2.*FI)*(N*(2*N-1)*T16+(N-2)*T3)
  H12=DKK*X*Y*B2*(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)
  H12R=(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*(2.*X*Y*B2/RAD(1)
&+X*Y*B2R)*DKK
  H12S=(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*(2.*Z*X*Y*B2/DY
&+X*Y*B2S)*DKK
  H12F=DKK*(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*DY**2.*B2*
&DCOS(2.*FI)
  H12C=DKK*X*Y*B2*(-1.*N*(2*N-1)*CC*T14+(N+1)*(N-2)*T17)
  H12CR=(-1.*N*(2*N-1)*CC*T14+(N+1)*(N-2)*T17)*(2.*X*Y*B2/RAD(1)
&+X*Y*B2R)*DKK
  H12CS=(-1.*N*(2*N-1)*CC*T14+(N+1)*(N-2)*T17)*(2.*Z*X*Y*B2/DY
&+X*Y*B2S)*DKK
  H12CF=DKK*(-1.*N*(2*N-1)*CC*T14+(N+1)*(N-2)*T17)*DY**2.*B2*
&DCOS(2.*FI)
  H13=.5*X*Y*B2*(F7-N*(N+1)*F18/(-BB)**2.)
  H13R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(F7-N*(N+1)*F18/(-BB)**2.)
  H13S=(2.*X*Y*Z*B2/DY+X*Y*B2S)*(F7-N*(N+1)*F18/(-BB)**2.)
  H13F=DY**2.*B2*DCOS(2.*FI)*(F7-N*(N+1)*F18/(-BB)**2.)
  H13C=.5*X*Y*B2*(T7-N*(N+1)*T18/CC**2.)
  H13CR=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(T7-N*(N+1)*T18/CC**2.)
  H13CS=(2.*X*Y*Z*B2/DY+X*Y*B2S)*(T7-N*(N+1)*T18/CC**2.)
  H13CF=DY**2.*B2*DCOS(2.*FI)*(T7-N*(N+1)*T18/CC**2.)
  H14=-1.*X*Y*B2*F7
  H14R=-1.*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F7
  H14S=-1.*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F7
  H14F=-1.*DY**2.*B2*DCOS(2.*FI)*F7
  H14C=-1.*X*Y*B2*T7
  H14CR=-1.*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*T7
  H14CS=-1.*(2.*X*Y*Z*B2/DY+X*Y*B2S)*T7
  H14CF=-1.*DY**2.*B2*DCOS(2.*FI)*T7
  H15=N*DKK*X*Y*B2*F19
  H15R=N*DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F19
  H15S=N*DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F19
  H15F=N*DKK*DY**2.*B2*DCOS(2.*FI)*F19
  H15C=N*DKK*X*Y*B2*T19
  H15CR=N*DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*T19
  H15CS=N*DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*T19
  H15CF=N*DKK*DY**2.*B2*DCOS(2.*FI)*T19
  H16=-.5*X*Y*B2*(F11+N*(N+1)*F20/(-BB)**2.)
```

```
  H16R=-.5*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16S=-.5*(2.*X*Y*Z*B2/DY+X*Y*B2S)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16F=-.5*DY**2.*B2*DCOS(2.*FI)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16C=-.5*X*Y*B2*(T11+N*(N+1)*T20/CC**2.)
  H16CR=-.5*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(T11+N*(N+1)*T20/CC**2.)
  H16CS=-.5*(2.*X*Y*Z*B2/DY+X*Y*B2S)*(T11+N*(N+1)*T20/CC**2.)
  H16CF=-.5*DY**2.*B2*DCOS(2.*FI)*(T11+N*(N+1)*T20/CC**2.)
  H17=X*Y*B2*F11
  H17R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F11
  H17S=(2.*X*Y*Z*B2/DY+X*Y*B2S)*F11
  H17F=DY**2.*B2*DCOS(2.*FI)*F11
  H17C=X*Y*B2*T11
  H17CR=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*T11
  H17CS=(2.*X*Y*Z*B2/DY+X*Y*B2S)*T11
  H17CF=DY**2.*B2*DCOS(2.*FI)*T11
  H18=DKK*X*Y*B2*F14
  H18R=DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F14
  H18S=DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F14
  H18F=DKK*DY**2.*B2*DCOS(2.*FI)*F14
  H18C=DKK*X*Y*B2*T14
  H18CR=DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*T14
  H18CS=DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*T14
  H18CF=DKK*DY**2.*B2*DCOS(2.*FI)*T14
  H19=-1.*X*AJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*
&F15/(-BB)**2.)/DKK**2./DY
  H19R=-1.*X*PAJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*
&F15/(-BB)**2.)/DKK/RAD(1)
  H19S=-1.*X*Z*PAJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*
&(N-2)*F15/(-BB)**2.)/DKK/DY
  H19F=Y*AJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*F15
&/(-BB)**2.)/DKK**2./DY
  H19C=-1.*X*AJ1*(N*(2*N-1)*(T14-T16)-.5*(N-2)*T3-.5*N*(N+1)*(N-2)*
&T15/CC**2.)/DKK**2./DY
  H19CR=-1.*X*PAJ1*(N*(2*N-1)*(T14-T16)-.5*(N-2)*T3-.5*N*(N+1)*(N-2)
&*T15/CC**2.)/DKK/RAD(1)
  H19CS=-1.*X*Z*PAJ1*(N*(2*N-1)*(T14-T16)-.5*(N-2)*T3-.5*N*(N+1)*
&(N-2)*T15/CC**2.)/DKK/DY
  H19CF=Y*AJ1*(N*(2*N-1)*(T14-T16)-.5*(N-2)*T3-.5*N*(N+1)*(N-2)*T15
&/CC**2.)/DKK**2./DY
  H20=-1.*X*AJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DKK/DY
  H20R=-1.*X*PAJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/RAD(1)
  H20S=-1.*X*Z*PAJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DY
  H20F=Y*AJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DY/DKK
  H20C=-1.*X*AJ1*(N*(2*N-1)*CC*T14-(N+1)*(N-2)*T17)/DKK/DY
  H20CR=-1.*X*PAJ1*(N*(2*N-1)*CC*T14-(N+1)*(N-2)*T17)/RAD(1)
  H20CS=-1.*X*Z*PAJ1*(N*(2*N-1)*CC*T14-(N+1)*(N-2)*T17)/DY
  H20CF=Y*AJ1*(N*(2*N-1)*CC*T14-(N+1)*(N-2)*T17)/DY/DKK
  H21=-.5*X*AJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DKK**2./DY
  H21R=-.5*X*PAJ1*(F7+N*(N+1)*F18/(-BB)**2.)/RAD(1)/DKK
  H21S=-.5*X*Z*PAJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DY/DKK
  H21F=.5*Y*AJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DY/DKK**2.
  H21C=-.5*X*AJ1*(T7+N*(N+1)*T18/CC**2.)/DKK**2./DY
  H21CR=-.5*X*PAJ1*(T7+N*(N+1)*T18/CC**2.)/RAD(1)/DKK
  H21CS=-.5*X*Z*PAJ1*(T7+N*(N+1)*T18/CC**2.)/DY/DKK
  H21CF=.5*Y*AJ1*(T7+N*(N+1)*T18/CC**2.)/DY/DKK**2.
  H22=N*X*AJ1*F19/DKK/DY
  H22R=N*X*PAJ1*F19/RAD(1)
  H22S=N*X*Z*PAJ1*F19/DY
```

```
  H22F=-1.*N*Y*AJ1*F19/DY/DKK
  H22C=N*X*AJ1*T19/DKK/DY
  H22CR=N*X*PAJ1*T19/RAD(1)
  H22CS=N*X*Z*PAJ1*T19/DY
  H22CF=-1.*N*Y*AJ1*T19/DY/DKK
  H23=.5*X*AJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DKK**2./DY
  H23R=.5*X*PAJ1*(F11-N*(N+1)*F20/(-BB)**2.)/RAD(1)/DKK
  H23S=.5*X*Z*PAJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DY/DKK
  H23F=-.5*Y*AJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DY/DKK**2.
  H23C=.5*X*AJ1*(T11-N*(N+1)*T20/CC**2.)/DKK**2./DY
  H23CR=.5*X*PAJ1*(T11-N*(N+1)*T20/CC**2.)/RAD(1)/DKK
  H23CS=.5*X*Z*PAJ1*(T11-N*(N+1)*T20/CC**2.)/DY/DKK
  H23CF=-.5*Y*AJ1*(T11-N*(N+1)*T20/CC**2.)/DY/DKK**2.
  H24=X*AJ1*F14/DKK/DY
  H24R=X*PAJ1*F14/RAD(1)
  H24S=X*Z*PAJ1*F14/DY
  H24F=-1.*Y*AJ1*F14/DY/DKK
  H24C=X*AJ1*T14/DKK/DY
  H24CR=X*PAJ1*T14/RAD(1)
  H24CS=X*Z*PAJ1*T14/DY
  H24CF=-1.*Y*AJ1*T14/DY/DKK
  ANN1(II)=WET(II)*(G5*H1+G6*H2+G1*H3-D5*H1C-D6*H2C-D1*H3C)*
&DEXP(DKK)
  ANN1R(II)=WET(II)*(G5R*H1+G5*H1R+G6R*H2+G6*H2R+G1R*H3
&+G1*H3R
&-D5R*H1C-D5*H1CR-D6R*H2C-D6*H2CR-D1R*H3C-D1*H3CR)
&*DEXP(DKK)
  ANN1S(II)=WET(II)*(G5S*H1+G5*H1S+G6S*H2+G6*H2S+G1S*H3
&+G1*H3S
&-D5S*H1C-D5*H1CS-D6S*H2C-D6*H2CS-D1S*H3C-D1*H3CS)
&*DEXP(DKK)
  ANN1F(II)=WET(II)*(G5*H1F+G6*H2F+G1*H3F
&-D5*H1CF-D6*H2CF-D1*H3CF)*DEXP(DKK)
  BNN1(II)=WET(II)*(G5*H4+G6*H5+G1*H6-
&D5*H4C-D6*H5C-D1*H6C)*DEXP(DKK)
  BNN1R(II)=WET(II)*(G5R*H4+G5*H4R+G6R*H5+G6*H5R
&+G1R*H6+G1*H6R
&-D5R*H4C-D5*H4CR-D6R*H5C-D6*H5CR-D1R*H6C-D1*H6CR)
&*DEXP(DKK)
  BNN1S(II)=WET(II)*(G5S*H4+G5*H4S+G6S*H5+G6*H5S+G1S*H6
&+G1*H6S
& -D5S*H4C-D5*H4CS-D6S*H5C-D6*H5CS-D1S*H6C-D1*H6CS)
& *DEXP(DKK)
  BNN1F(II)=WET(II)*(G5*H4F+G6*H5F+G1*H6F-
&D5*H4CF-D6*H5CF-D1*H6CF)*DEXP(DKK)
  CNN1(II)=WET(II)*(G5*H7+G6*H8+G1*H9-
&D5*H7C-D6*H8C-D1*H9C)*DEXP(DKK)
  CNN1R(II)=WET(II)*(G5R*H7+G5*H7R+G6R*H8+G6*H8R
&+G1R*H9+G1*H9R
&-D5R*H7C-D5*H7CR-D6R*H8C-D6*H8CR-D1R*H9C-D1*H9CR)
&*DEXP(DKK)
  CNN1S(II)=WET(II)*(G5S*H7+G5*H7S+G6S*H8
&+G6*H8S+G1S*H9+G1*H9S
&-D5S*H7C-D5*H7CS-D6S*H8C-D6*H8CS-D1S*H9C-D1*H9CS)
&*DEXP(DKK)
  CNN1F(II)=WET(II)*(G5*H7F+G6*H8F+G1*H9F-
&D5*H7CF-D6*H8CF-D1*H9CF)*DEXP(DKK)
  ANN2(II)=WET(II)*(G6*H10+G3*H11+G1*H12-
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     &D6*H10C-D3*H11C-D1*H12C)*DEXP(DKK)
      ANN2R(II)=WET(II)*(G6R*H10+G6*H10R+G3R*H11
     &+G3*H11R+G1R*H12+G1*
     &H12R-D6R*H10C-D6*H10CR-D3R*H11C-D3*H11CR-D1R*H12C-D1*
     &H12CR)*DEXP(DKK)
      ANN2S(II)=WET(II)*(G6S*H10+G6*H10S+G3S*H11
     &+G3*H11S+G1S*H12+G1*
     &H12S-D6S*H10C-D6*H10CS-D3S*H11C-D3*H11CS-D1S*H12C-D1*
     &H12CS)*DEXP(DKK)
      ANN2F(II)=WET(II)*(G6*H10F+G3*H11F+G1*H12F-
     &D6*H10CF-D3*H11CF-D1*H12CF)*DEXP(DKK)
      BNN2(II)=WET(II)*(G6*H13+G3*H14+G1*H15-
     &D6*H13C-D3*H14C-D1*H15C)*DEXP(DKK)
      BNN2R(II)=WET(II)*(G6R*H13+G6*H13R+G3R*H14
     &+G3*H14R+G1R*H15+G1*
     &H15R-D6R*H13C-D6*H13CR-D3R*H14C-D3*H14CR-D1R*H15C-D1*
     &H15CR)*DEXP(DKK)
      BNN2S(II)=WET(II)*(G6S*H13+G6*H13S+G3S*H14
     &+G3*H14S+G1S*H15+G1*
     &H15S-D6S*H13C-D6*H13CS-D3S*H14C-D3*H14CS-D1S*H15C-D1*
     &H15CS)*DEXP(DKK)
      BNN2F(II)=WET(II)*(G6*H13F+G3*H14F+G1*H15F-
     &D6*H13CF-D3*H14CF-D1*H15CF)*DEXP(DKK)
      CNN2(II)=WET(II)*(G6*H16+G3*H17+G1*H18-
     &D6*H16C-D3*H17C-D1*H18C)*DEXP(DKK)
      CNN2R(II)=WET(II)*(G6R*H16+G6*H16R+G3R*H17
     &+G3*H17R+G1R*H18+G1*
     &H18R-D6R*H16C-D6*H16CR-D3R*H17C-D3*H17CR-D1R*H18C-D1*
     &H18CR)*DEXP(DKK)
      CNN2S(II)=WET(II)*(G6S*H16+G6*H16S+G3S*H17
     &+G3*H17S+G1S*H18+G1*
     &H18S-D6S*H16C-D6*H16CS-D3S*H17C-D3*H17CS-D1S*H18C-D1*
     &H18CS)*DEXP(DKK)
      CNN2F(II)=WET(II)*(G6*H16F+G3*H17F+G1*H18F-
     &D6*H16CF-D3*H17CF-D1*H18CF)*DEXP(DKK)
      ANN3(II)=WET(II)*(G2*H19+G4*H20-D2*H19C-D4*H20C)*DEXP(DKK)
      ANN3R(II)=WET(II)*(G2R*H19+G2*H19R+G4R*H20+G4*H20R-
     &D2R*H19C-D2*H19CR-D4R*H20C-D4*H20CR)*DEXP(DKK)
      ANN3S(II)=WET(II)*(G2S*H19+G2*H19S+G4S*H20+G4*H20S-
     &D2S*H19C-D2*H19CS-D4S*H20C-D4*H20CS)*DEXP(DKK)
      ANN3F(II)=WET(II)*(G2*H19F+G4*H20F-D2*H19CF-
     &D4*H20CF)*DEXP(DKK)
      BNN3(II)=WET(II)*(G2*H21+G4*H22-D2*H21C-D4*H22C)*DEXP(DKK)
      BNN3R(II)=WET(II)*(G2R*H21+G2*H21R+G4R*H22+G4*H22R-
     &D2R*H21C-D2*H21CR-D4R*H22C-D4*H22CR)*DEXP(DKK)
      BNN3S(II)=WET(II)*(G2S*H21+G2*H21S+G4S*H22+G4*H22S-
     &D2S*H21C-D2*H21CS-D4S*H22C-D4*H22CS)*DEXP(DKK)
      BNN3F(II)=WET(II)*(G2*H21F+G4*H22F-D2*H21CF-
     &D4*H22CF)*DEXP(DKK)
      CNN3(II)=WET(II)*(G2*H23+G4*H24-D2*H23C-D4*H24C)*DEXP(DKK)
      CNN3R(II)=WET(II)*(G2R*H23+G2*H23R+G4R*H24+G4*H24R-
     &D2R*H23C-D2*H23CR-D4R*H24C-D4*H24CR)*DEXP(DKK)
      CNN3S(II)=WET(II)*(G2S*H23+G2*H23S+G4S*H24+G4*H24S-
     &D2S*H23C-D2*H23CS-D4S*H24C-D4*H24CS)*DEXP(DKK)
      CNN3F(II)=WET(II)*(G2*H23F+G4*H24F-D2*H23CF-
     &D4*H24CF)*DEXP(DKK)
2001  CONTINUE
      SUM1=0.D0
```

```
SUM2=0.D0
SUM3=0.D0
SUM4=0.D0
SUM5=0.D0
SUM6=0.D0
SUM7=0.D0
SUM8=0.D0
SUM9=0.D0
SUM10=0.D0
SUM11=0.D0
SUM12=0.D0
SUM13=0.D0
SUM14=0.D0
SUM15=0.D0
SUM16=0.D0
SUM17=0.D0
SUM18=0.D0
SUM19=0.D0
SUM20=0.D0
SUM21=0.D0
SUM22=0.D0
SUM23=0.D0
SUM24=0.D0
SUM25=0.D0
SUM26=0.D0
SUM27=0.D0
SUM28=0.D0
SUM29=0.D0
SUM30=0.D0
SUM31=0.D0
SUM32=0.D0
SUM33=0.D0
SUM34=0.D0
SUM35=0.D0
SUM36=0.D0
DO 1999 IJ=1,IN
SUM1=SUM1+ANN1(IJ)
SUM2=SUM2+ANN2(IJ)
SUM3=SUM3+ANN3(IJ)
SUM4=SUM4+BNN1(IJ)
SUM5=SUM5+BNN2(IJ)
SUM6=SUM6+BNN3(IJ)
SUM7=SUM7+CNN1(IJ)
SUM8=SUM8+CNN2(IJ)
SUM9=SUM9+CNN3(IJ)
SUM10=SUM10+ANN1R(IJ)
SUM11=SUM11+ANN2R(IJ)
SUM12=SUM12+ANN3R(IJ)
SUM13=SUM13+BNN1R(IJ)
SUM14=SUM14+BNN2R(IJ)
SUM15=SUM15+BNN3R(IJ)
SUM16=SUM16+CNN1R(IJ)
SUM17=SUM17+CNN2R(IJ)
SUM18=SUM18+CNN3R(IJ)
SUM19=SUM19+ANN1S(IJ)
SUM20=SUM20+ANN2S(IJ)
SUM21=SUM21+ANN3S(IJ)
SUM22=SUM22+BNN1S(IJ)
```

```
      SUM23=SUM23+BNN2S(IJ)
      SUM24=SUM24+BNN3S(IJ)
      SUM25=SUM25+CNN1S(IJ)
      SUM26=SUM26+CNN2S(IJ)
      SUM27=SUM27+CNN3S(IJ)
      SUM28=SUM28+ANN1F(IJ)
      SUM29=SUM29+ANN2F(IJ)
      SUM30=SUM30+ANN3F(IJ)
      SUM31=SUM31+BNN1F(IJ)
      SUM32=SUM32+BNN2F(IJ)
      SUM33=SUM33+BNN3F(IJ)
      SUM34=SUM34+CNN1F(IJ)
      SUM35=SUM35+CNN2F(IJ)
      SUM36=SUM36+CNN3F(IJ)
1999  CONTINUE
      RETURN
      END

      SUBROUTINE BEST(N,M,J,L,ABK,ZZ1,BBB)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PI=DACOS(-1.D0)
      FFD=0.D0
      DO 104 IQ=0,INT(N/2)
      IF (N-2*IQ-M .LT. 0) THEN
      FFD1=0.D0
      GO TO 1435
      ELSE
      CALL GAMMA(N-2*IQ-M,AA1)
      CALL GAMMA(IQ,AA2)
      XZ=ABK*ABS(ZZ1)
      FFD1=((2/PI)**.5)/((-2.D0)**IQ)/AA2/AA1/(ZZ1)**(N+M)
      END IF
      CALL AKV(N,IQ,J,XZ,WK)
1435  CONTINUE
      FFD=FFD+FFD1*WK*(ABK*ABS(ZZ1))**(N-IQ+L-.5)
104   CONTINUE
      BBB=FFD
      IF (N .LT. M) THEN
      BBB=0.D0
      END IF
      RETURN
      END

      SUBROUTINE AKV(N,IQ,J,X,FDK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION AAK(-20:80),FFK(-20:80)
      IF (N-IQ-J .GE. 1) THEN
      NN=N-IQ-J-1
      ELSE
      NN=N-IQ-J
      END IF
      PI=DACOS(-1.D0)
      AAK(0)=-1.*(.5D0*PI/X)/DEXP(X)
      AAK(1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      AAK(-1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(-2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(0)=(.5D0*PI/X)**.5/DEXP(X)
```

```
      FFK(1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(-1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(-2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      IF (IABS(NN) .LE. 2 ) THEN
      GO TO 2233
      END IF
      DO 502 I=3,IABS(NN)
      AAK(I)=AAK(I-2)-(2*I-1)*AAK(I-1)/X
      FFK(I)=AAK(I)/(-1.)**(I+1)/(.5*PI/X)**.5
      FFK(-I)=FFK(I)
502   CONTINUE
2233  CONTINUE
      FDK=FFK(NN)
4443  CONTINUE
      RETURN
      END

      SUBROUTINE GAMMA(J,AJK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IF (J .EQ. 0) THEN
      AJK=1.D0
      ELSE
      AJK=1.D0
      DO 300 I=1,J
      SS=DBLE(I)
      AJK=AJK*SS
300   CONTINUE
      END IF
      RETURN
      END

      SUBROUTINE BESSEL(CX,AJ,AJ0,AJ1,AJ2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      AJ0=0.D0
      AJ1=0.D0
      AJ2=0.D0
      DO 100 J=0,50
      CALL GAMMA(J,AJK)
      TJ=AJ0
      AJ0=AJ0+((-1.D0)**J)*(CX/2.)**(2*J)/(AJK)**2.
      IF (ABS(AJ0-TJ) .LE. 0.000000000000001 ) THEN
      GO TO    500
      END IF
100   CONTINUE
500   CONTINUE
      DO 107 J=0,50
      CALL GAMMA(J,AJK)
      TJ1=AJ1
      AJ1=AJ1+((-1.D0)**J)*(CX/2.)**(2*J+1)/((AJK)**2.)/(J+1)
      IF (ABS(AJ1-TJ1) .LE. 0.000000000000001 ) THEN
      GO TO 201
      END IF
107   CONTINUE
201   CONTINUE
      DO 108 J=0,50
      CALL GAMMA(J,AJK)
      TJ2=AJ2
```

```
      AJ2=AJ2+((-1.D0)**J)*(CX/2.)**(2*J+2)/((AJK)**2.)/(J+1)
     &/(J+2)
      IF (ABS(AJ2-TJ2)    .LE. 0.0000000000000001) THEN
      GO TO 200
      END IF
108   CONTINUE
200   CONTINUE
      AJ=-1.*AJ1
      RETURN
      END

      SUBROUTINE XRD(N,BB,CC,IN,
     &RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN(96),RAD(2),AN1(96),AN2(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      E2=DDK(II)*(ZZ-CC)
      E1=DDK(II)*(BB+CC)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      CALL BEST(N+1,1,1,0,DKK,-BB,VV1)
      CALL BEST (N+1,1,1,0,DKK,CC,VV2)
      AN(II)=WET(II)*N*((CC)**2.*DCOSH(E3)*AJ1*VV2/DSINH(E1)-
     &(-BB)**2.*AJ1*VV1*DCOSH(E2)/DSINH(E1))*DEXP(DKK)
      AN1(II)=WET(II)*N*(DKK*CC**2.*U2*DSINH(E3)*AJ1*U4*VV2/DSINH(
     &E1)+DKK*CC**2.*U3*DCOSH(E3)*PAJ1*VV2*U4/DSINH(E1)-DKK*
     &(-BB)**2.*U2*DSINH(E2)*AJ1*VV1*U4/DSINH(E1)-DKK*(-BB)**2.*U3
     &*DCOSH(E2)*PAJ1*VV1*U4/DSINH(E1))*DEXP(DKK)
      AN2(II)=WET(II)*N*(-DKK*CC**2.*RAD(1)*U3*DSINH(E3)*AJ1*U4*VV2/
     &DSINH(E1)+DKK*CC**2.*RAD(1)*U2*DCOSH(E3)*PAJ1*VV2*U4
     &/DSINH(E1)
     &+DKK*(-BB)**2.*RAD(1)*U3*DSINH(E2)*AJ1*VV1*U4/DSINH(E1)-
     &DKK*(-BB)**2.*RAD(1)*U2*DCOSH(E2)*PAJ1*VV1*U4/DSINH(E1))*
     &DEXP(DKK)
2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN(IJ)
      SM2=SM2+AN1(IJ)
      SM3=SM3+AN2(IJ)
1999  CONTINUE
      RETURN
      END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                    FOR LINEAR TEMPERATURE PROFILE                    C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


      SUBROUTINE XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN(96),RAD(2),AN1(96),AN2(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      E2=DDK(II)*(ZZ-CC)
      E1=DDK(II)*(BB+CC)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      CALL BEST(N,1,1,0,DKK,-BB,VV1)
      CALL BEST (N,1,1,0,DKK,CC,VV2)
      AN(II)=WET(II)*(-DKK*(CC)**2.*DSINH(E3)*AJ1*VV2/DSINH(E1)+DKK*
     & (-BB)**2.*AJ1*VV1*DSINH(E2)/DSINH(E1))*DEXP(DKK)
      AN1(II)=WET(II)*(-DKK**2.*CC**2.*U2*DCOSH(E3)*AJ1*U4*VV2/DSINH(
     & E1)-DKK**2.*CC**2.*U3*DSINH(E3)*PAJ1*VV2*U4/DSINH(E1)+DKK**2.*
     & (-BB)**2.*U2*DCOSH(E2)*AJ1*VV1*U4/DSINH(E1)+DKK**2.*(-BB)**2.*U3
     & *DSINH(E2)*PAJ1*VV1*U4/DSINH(E1))*DEXP(DKK)

      AN2(II)=WET(II)*(DKK**2.*CC**2.*RAD(1)*U3*DCOSH(E3)*AJ1*U4*VV2/
     &DSINH(E1)-DKK**2.*CC**2.*RAD(1)*U2*DSINH(E3)*PAJ1*VV2*U4/DSINH(E1)
     &-DKK**2.*(-BB)**2.*RAD(1)*U3*DCOSH(E2)*AJ1*VV1*U4/DSINH(E1)+
     &DKK**2.*(-BB)**2.*RAD(1)*U2*DSINH(E2)*PAJ1*VV1*U4/DSINH(E1))*
     & DEXP(DKK)

2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN(IJ)
      SM2=SM2+AN1(IJ)
      SM3=SM3+AN2(IJ)
1999  CONTINUE
      RETURN
      END
```

Appendix E4-1: Computer programming source code for estimating the thermophoretic velocity of one spherical colloid parallel one insulated plate.

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      REAL*8 CONST1,CONST2
      DIMENSION A(500,501),RAD(2),DDK(96),WET(96),B(500,501),BF(500,3)
      INTEGER T,GG,LL1,LL2,LBB,LCC,GGG
      OPEN (23,FILE='GAUSS80.DAT',STATUS='OLD')
      OPEN (24,FILE='WET3.DAT',STATUS='OLD')
      OPEN (25,FILE='DTTH0.2-0.1-0.DAT',STATUS='NEW')
      IN=80
      BB=0.1D0
      ETK=0.D0
      DO 1001 I=1,IN
      READ (23,*) DDK(I),WET(I)
1001  CONTINUE
      T=1
      PI=DACOS(-1.D0)
      FI=.01*PI/180.
      U4=DCOS(FI)
      U5=DSIN(FI)
      DO 3231    IUY=1,50
      READ (24,*) CV,NX
      RAD(1)=CV*BB
      CONST1=0.2D0*RAD(1)
      CONST2=0.1D0*RAD(1)
      GGG=2*NX
      DO 511 I=1,T
      DO 512 J=1,NX
      NU=J+NX*(I-1)
      NY=J+NX*(I-1)+T*NX
      DO 513 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      B(NU,GGG+1)=-1.*RAD(1)*U3+U3*CONST1
      B(NY,GGG+1)=-1.*U3
      DO 514 N=1,NX
      NZ=(2*N-1)+2*NX*(K-1)
      NL=2*N+2*NX*(K-1)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      B(NU,NZ)=R2**(-N-1)*W1+SM1-(SM2-(N+1)*R2**(-N-2)*W1)*CONST1
      B(NU,NL)=-R2**N*W1
      B(NY,NZ)=(-N-1)*R2**(-N-2)*W1+SM2
      B(NY,NL)=-ETK*N*R2**(N-1)*W1

514   CONTINUE
513   CONTINUE
```

```
512     CONTINUE
511     CONTINUE

        LL1=500
        LL2=501
        LBB=GGG
        LCC=GGG+1
        CALL GAUSL (LL1,LL2,LBB,LCC,B)
        GG=T*NX
        DO 7765 NN=1,3
        DO 111 I=1,T
        DO 112 J=1,NX
        NA=J+NX*(I-1)
        NB=J+NX*(I-1)+T*NX
        NC=J+NX*(I-1)+2*T*NX
        DO 113 K=1,T
        CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)

        IF (NN .EQ. 1) THEN
        A(NA,3*GG+1)=U3*U4
        A(NB,3*GG+1)=U2*U4
        A(NC,3*GG+1)=-1.*U5
        END IF

        IF(NN .EQ. 2) THEN
        A(NA,3*GG+1)=0.D0
        A(NB,3*GG+1)=U4
        A(NC,3*GG+1)=-1.*U2*U5
        END IF

        DO 114 N=1,NX
        NE=(3*N-2)+3*NX*(K-1)
        NG=(3*N-1)+3*NX*(K-1)
        NI=(3*N-0)+3*NX*(K-1)

        CALL FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
        CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
        CALL FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
        CALL XXD(FI,N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SUM1,SUM2,SUM3
       &,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9,SUM10,SUM11,SUM12,SUM13,SUM14
       &,SUM17,SUM18,SUM19,SUM20,SUM21,SUM22,SUM23,SUM24,SUM25,SUM26,
       & SUM27,SUM28,SUM29,SUM30,SUM31,SUM32,SUM33,SUM34,SUM35,SUM36
       & ,SUM15,SUM16)
        AA1=((2.*N*(2*N-1)*U3*W1*U4**2.+(N-2)*WW2*DCOS(2.*FI)-N*(N+1)
       &*(N-2)*WW)/2./R2**(N))
        BB1=-1.*(WWW2*DCOS(2.*FI)-N*(N+1)*WWW)/2./R2**(N+2)
        CC1=(W2*DCOS(2.*FI)+N*(N+1)*W)/2./R2**(N+1)
        AA2=(N*(2*N-1)*U3*W1+(N-2)*WW2)*U4*U5/R2**(N)
        BB2=-1.*(WWW2*U4*U5)/R2**(N+2)
```

```
  CC2=(W2*U4*U5)/R2**(N+1)
  AA3=(N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U4/R2**N
  BB3=-1.*(N*WWW1*U4)/R2**(N+2)
  CC3=-1.*(W1*U4)/R2**(N+1)

  AA1R=-1.*N*AA1/R2
  BB1R=-1.*(N+2)*BB1/R2
  CC1R=-1.*(N+1)*CC1/R2
  AA2R=-1.*N*AA2/R2
  BB2R=-1.*(N+2)*BB2/R2
  CC2R=-1.*(N+1)*CC2/R2
  AA3R=-1.*N*AA3/R2
  BB3R=-1.*(N+2)*BB3/R2
  CC3R=-1.*(N+1)*CC3/R2

  AA1S=(2.*N*(2*N-1)*U2*W1*U4**2.-2.*N*(2*N-1)*U3**2.*PW1*U4**2.-
*(N-2)*U3*PWW2*DCOS(2.*FI)+N*(N+1)*(N-2)*U3*PWW)/2./R2**N
  BB1S=-1.*(-1.*U3*PWWW2*DCOS(2.*FI)+N*(N+1)*U3*PWWW)/2./R2**(N+2)
  CC1S=(-1.*U3*PW2*DCOS(2.*FI)-U3*N*(N+1)*PW)/2./R2**(N+1)
  AA2S=(U2*N*(2*N-1)*W1-N*(2*N-1)*U3**2.*PW1-U3*(N-2)*PWW2)*U4*
&U5/R2**N
  BB2S=(U3*PWWW2*U4*U5)/R2**(N+2)
  CC2S=(-1.*U3*PW2*U4*U5)/R2**(N+1)
  AA3S=(-1.*N*(2.*N-1)*U3*W1-U2*U3*N*(2*N-1)*PW1+U3*(N+1)*(N-2)
&*PWW1)*U4/R2**N
  BB3S=U3*N*PWWW1*U4/R2**(N+2)
  CC3S=U3*PW1*U4/R2**(N+1)
  AA1F=((-2.*N*(2*N-1)*U3*W1*U4*U5-(N-2)*WW2*DSIN(2.*FI)
* )/R2**(N))
  BB1F=WWW2*DSIN(2.*FI)/R2**(N+2)
  CC1F=-1.*W2*DSIN(2.*FI)/R2**(N+1)
  AA2F=(N*(2*N-1)*U3*W1+(N-2)*WW2)*DCOS(2.*FI)/R2**(N)
  BB2F=-1.*(WWW2*DCOS(2.*FI))/R2**(N+2)
  CC2F=(W2*DCOS(2.*FI))/R2**(N+1)
  AA3F=-1.*(N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U5/R2**N
  BB3F=(N*WWW1*U5)/R2**(N+2)
  CC3F=(W1*U5)/R2**(N+1)
  A(NA,NE)=U3*U4*(AA1+SUM1)+U3*U5*(AA2+SUM2)+U2*(AA3+SUM3)
  A(NA,NG)=U3*U4*(BB1+SUM4)+U3*U5*(BB2+SUM5)+U2*(BB3+SUM6)
  A(NA,NI)=U3*U4*(CC1+SUM7)+U3*U5*(CC2+SUM8)+U2*(CC3+SUM9)
  A(NB,NE)=(U2*U4*(AA1+SUM1)+U2*U5*(AA2+SUM2)-U3*(AA3+SUM3))
&-CONST2*(U2*U4*(AA1R+SUM10)+U2*U5*(AA2R+SUM11)-U3*(AA3R+SUM12)
&+(U3*U4*(AA1S+SUM19)+U3*U5*(AA2S+SUM20)+U2*(AA3S+SUM21))/R2)
  A(NB,NG)=(U2*U4*(BB1+SUM4)+U2*U5*(BB2+SUM5)-U3*(BB3+SUM6))
  &-CONST2*(U2*U4*(BB1R+SUM13)+U2*U5*(BB2R+SUM14)-U3*(BB3R+SUM15)
&+(U3*U4*(BB1S+SUM22)+U3*U5*(BB2S+SUM23)+U2*(BB3S+SUM24))/R2)
  A(NB,NI)=(U2*U4*(CC1+SUM7)+U2*U5*(CC2+SUM8)-U3*(CC3+SUM9))
&-CONST2*(U2*U4*(CC1R+SUM16)+U2*U5*(CC2R+SUM17)-U3*(CC3R+SUM18)
&+(U3*U4*(CC1S+SUM25)+U3*U5*(CC2S+SUM26)+U2*(CC3S+SUM27))/R2)
```

```
      A(NC,NE)=(-1.*U5*(AA1+SUM1)+U4*(AA2+SUM2))
     &-CONST2*(-1.*U5*(AA1R+SUM10)+U4*(AA2R+SUM11)+(U4*(AA1F+SUM28)+
     &U5*(AA2F+SUM29)+U2*(AA3F+SUM30)/U3)/R2)
      A(NC,NG)=(-1.*U5*(BB1+SUM4)+U4*(BB2+SUM5))
     &-CONST2*(-1.*U5*(BB1R+SUM13)+U4*(BB2R+SUM14)+(U4*(BB1F+SUM31)+
     &U5*(BB2F+SUM32)+U2*(BB3F+SUM33)/U3)/R2)
      A(NC,NI)=(-1.*U5*(CC1+SUM7)+U4*(CC2+SUM8))
     &-CONST2*(-1.*U5*(CC1R+SUM16)+U4*(CC2R+SUM17)+(U4*(CC1F+SUM34)+
     &U5*(CC2F+SUM35)+U2*(CC3F+SUM36)/U3)/R2)
114   CONTINUE
113   CONTINUE
112   CONTINUE
111   CONTINUE

        IF (NN .EQ. 3) THEN
        DO 811 J=1,NX
        NA=J
        NB=J+NX
        NC=J+2*NX
        CALL FU(1,J,1,NX,RAD,PI,U2,U3,R2)
        VALUE=0.D0
        VALUE1=0.D0
        DO 713 KK=1,NX
        NZ=2*KK-1
        CALL FUCK2(U2,KK,W1,WW1,WWW1,PW1,PWW1,PWWW1)
        CALL XRD(KK,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
        VALUE=VALUE+B(NZ,GGG+1)*(R2**(-KK-1)*PW1*U4*(-1.*U3)+U4*SM3)
        VALUE1=VALUE1+B(NZ,GGG+1)*(R2**(-KK-1)*W1*(-1.*U5)-U5*SM1)
713     CONTINUE
        A(NA,3*GG+1)=0.D0
        A(NB,3*GG+1)=(RAD(1)*U2*U4+VALUE)/RAD(1)
        A(NC,3*GG+1)=(-1.D0*RAD(1)*U3*U5+VALUE1)/(RAD(1)*U3)
811     CONTINUE
          END IF

      LL1=500
      LL2=501
      LBB=3*GG
      LCC=3*GG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,A)
      DO 999 I=1,3*GG
      BF(I,NN)=A(I,3*GG+1)
999   CONTINUE
7765  CONTINUE
      VVU=-2*(1+ETK*CONST1/RAD(1))/
     &((1+2*CONST2/RAD(1))*(2+ETK+2*ETK*CONST1/RAD(1)))
      HGD=-1*(BF(1,3)*BF(3,2)-BF(1,2)*BF(3,3))/
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      HGR=-1*(BF(1,1)*BF(3,3)-BF(1,3)*BF(3,1))/
```

```
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      XN=NX
      WRITE (*,9)CV,HGD,HGR,XN
      WRITE (25,9) CV,HGD,HGR,XN

3231  CONTINUE
9     FORMAT (6(F12.6))
      STOP
      END

      SUBROUTINE FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION RAD(2)
      PID=1.D-3
      DTHETA=(PI-4.D0*PID)/(NX-2)
      IF(J==1) THEN
      Z=RAD(I)*DCOS(PID)
      V=RAD(I)*DSIN(PID)
      END IF
      IF((1<J) .AND. (J<=NX/2)) THEN
      Z=RAD(I)*DCOS(PID+(J-1)*DTHETA)
      V=RAD(I)*DSIN(PID+(J-1)*DTHETA)
      END IF
      IF(NX/2<J) THEN
      Z=RAD(I)*DCOS(PI/2.D0+(J-1-NX/2)*DTHETA)
      V=RAD(I)*DSIN(PI/2.D0+(J-1-NX/2)*DTHETA)
      END IF
      U2=Z/RAD(I)
      U3=V/RAD(I)
      R2=RAD(I)
      RETURN
      END

      SUBROUTINE GAUSL (N,M,II,JJ,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(N,M)
      DO 10 I=1,II
      AA=0.E0
      DO 9 J=1,II
    9 AA=AA+ABS(A(I,J))
      DO 10 J=1,JJ
   10 A(I,J)=A(I,J)/AA
      CALL XXXXX (N,M,II,JJ-II,A)
      RETURN
      END

      SUBROUTINE XXXXX (ND,NCOL,N,NS,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(ND,NCOL)
```

```
      N1=N+1
      NT=N+NS
      IF(N.EQ.1) GO TO 50
      DO 10 I=2,N
      IP=I-1
      I1=IP
      X=ABS(A(I1,I1))
      DO 11 J=I,N
      IF(ABS(A(J,I1)).LT.X) GO TO 11
      X=ABS(A(J,I1))
      IP=J
   11 CONTINUE
      IF(IP.EQ.I1) GO TO 13
      DO 12 J=I1,NT
      X=A(I1,J)
      A(I1,J)=A(IP,J)
   12 A(IP,J)=X
   13 DO 10 J=I,N
      X=A(J,I1)/A(I1,I1)
      DO 10 K=I,NT
   10 A(J,K)=A(J,K)-X*A(I1,K)
   50 DO 20 IP=1,N
      I=N1-IP
      DO 20 K=N1,NT
      A(I,K)=A(I,K)/A(I,I)
      IF(I.EQ.1) GO TO 20
      I1=I-1
      DO 25 J=1,I1
   25 A(J,K)=A(J,K)-A(I,K)*A(J,I)
   20 CONTINUE
      RETURN
      END

      SUBROUTINE FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PA(-1:600)
      PA(-1)=0.D0
      PA(0)=0.D0
      PA(1)=(1.-U2**2)**.5
      PA(2)=3.*U2*(1.-U2**2)**.5
      DO 100 J=1,N+1
      PA(J+1)=((2*J+1)*U2*PA(J)-(J+1)*PA(J-1))/(J)
100   CONTINUE
      W1=PA(N)
      WW1=PA(N-1)
      WWW1=PA(N+1)
      PW1=(N*U2*PA(N)-(N+1)*PA(N-1))/(U2**2.-1.)
      PWW1=((N-1)*U2*PA(N-1)-(N)*PA(N-2))/(U2**2.-1.)
      PWWW1=((N+1)*U2*PA(N+1)-(N+2)*PA(N))/(U2**2.-1.)
```

```
      RETURN
      END

      SUBROUTINE FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PR(-1:600)
      PR(-1)=0.D0
      PR(0)=1.D0
      PR(1)=U2
      DO 34 I=2,N+1
      PR(I)=((2*I-1)*U2*PR(I-1)-(I-1)*PR(I-2))/I
34    CONTINUE
      W=PR(N)
      WW=PR(N-1)
      WWW=PR(N+1)
      PW=(N*U2*PR(N)-N*PR(N-1))/(U2**2.-1.)
      PWW=((N-1)*U2*PR(N-1)-(N-1)*PR(N-2))/(U2**2.-1.)
      PWWW=((N+1)*U2*PR(N+1)-(N+1)*PR(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PB(-1:600)
      PB(-1)=0.D0
      PB(0)=0.D0
      PB(1)=0.D0
      PB(2)=3.*(1.-U2**2)
      DO 150 K=2,N+1
      PB(K+1)=((2*K+1)*U2*PB(K)-(K+2)*PB(K-1))/(K-1)
150   CONTINUE
      W2=PB(N)
      WW2=PB(N-1)
      WWW2=PB(N+1)
      PW2=(N*U2*PB(N)-(N+2)*PB(N-1))/(U2**2.-1.)
      PWW2=((N-1)*U2*PB(N-1)-(N+1)*PB(N-2))/(U2**2.-1.)
      PWWW2=((N+1)*U2*PB(N+1)-(N+3)*PB(N))/(U2**2.-1.)
      RETURN
      END
      SUBROUTINE XXD(FI,N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SUM1,SUM2,SUM3
     &,SUM4,SUM5,SUM6,SUM7,SUM8,SUM9,SUM10,SUM11,SUM12,SUM13,SUM14
     &,SUM17,SUM18,SUM19,SUM20,SUM21,SUM22,SUM23,SUM24,SUM25,SUM26,
     & SUM27,SUM28,SUM29,SUM30,SUM31,SUM32,SUM33,SUM34,SUM35,SUM36
     & ,SUM15,SUM16)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),RAD(2)
      DIMENSION ANN1(96),ANN2(96),ANN3(96),BNN1(96),BNN2(96),BNN3(96)
      DIMENSION CNN1(96),CNN2(96),CNN3(96),ANN1R(96),ANN2R(96),ANN3R(96)
      DIMENSION BNN1R(96),BNN2R(96),BNN3R(96),CNN1R(96),CNN2R(96)
```

```
      DIMENSION CNN3R(96),ANN1S(96),ANN2S(96),ANN3S(96),BNN1S(96)
      DIMENSION BNN2S(96),BNN3S(96),CNN1S(96),CNN2S(96),CNN3S(96)
      DIMENSION ANN1F(96),ANN2F(96),ANN3F(96),BNN1F(96),BNN2F(96)
      DIMENSION BNN3F(96),CNN1F(96),CNN2F(96),CNN3F(96)
      DO 2001 II=1,IN
      Z=RAD(1)*U2
      X=RAD(1)*U3*U4
      Y=RAD(1)*U3*U5
      DKK=DDK(II)
      DY=RAD(1)*U3
      DDY=DKK*DY
      CALL BESSEL(DDY,AJ,AJ0,AJ1,AJ2)
      PAJ0=-1.*AJ1
      PAJ1=.5*(AJ0-AJ2)
      B1=AJ0*X**2.+(Y**2.-X**2.)*AJ1/DDY
      B2=(AJ0-2.*AJ1/DDY)/DDY**2.
      B1R=(X**2.*PAJ0*DDY+2.*X**2.*AJ0+(Y**2.-X**2.)*(AJ1+PAJ1*DDY)
     & /DDY)/RAD(1)
      B1S=Z*(X**2.*PAJ0*DDY+2.*X**2.*AJ0+(Y**2.-X**2.)*(AJ1+PAJ1*DDY
     & )/DDY)/DY
      B1F=-2.*X*Y*AJ0+4*X*Y*AJ1/DDY
      B2R=(6.*AJ1/DDY-2.*AJ0+DDY*PAJ0-2.*PAJ1)/RAD(1)/DDY**2.
      B2S=Z*(6.*AJ1/DDY-2.*AJ0+DDY*PAJ0-2.*PAJ1)/DDY**2./DY
      E3=DKK*(Z+BB)
      G5=DEXP(-1.*E3)
      G5R=-1.*DKK*U2*G5
      G5S=DKK*RAD(1)*U3*G5
      G6=-1.*E3*DEXP(-E3)
      G1=G6
      G6R=DKK*U2*(E3*G5-G5)
      G1R=G6R
      G6S=DKK*RAD(1)*U3*(G5-E3*G5)
      G1S=G6S
      G2=-1.*G6
      G2R=-1.*G6R
      G2S=-1.*G6S
      G3=(1.-E3)*G5
      G3R=DKK*U2*(E3*G5-2.*G5)
      G3S=DKK*RAD(1)*U3*(2.*G5-E3*G5)
      G4=(1.+E3)*G5
      G4R=-1.*DKK*U2*E3*G5
      G4S=DKK*RAD(1)*U3*E3*G5
      CALL BEST(N,1,1,0,DKK,-BB,F1)
      CALL BEST(N,1,2,1,DKK,-BB,F2)
      CALL BEST(N-1,2,2,3,DKK,-BB,F3)
      CALL BEST(N-1,0,0,1,DKK,-BB,F4)
      CALL BEST(N-1,2,2,1,DKK,-BB,F5)
      CALL BEST(N-1,1,1,0,DKK,-BB,F6)
      CALL BEST(N+1,2,2,3,DKK,-BB,F7)
```

```
  CALL BEST(N+1,0,0,1,DKK,-BB,F8)
  CALL BEST(N+1,2,2,1,DKK,-BB,F9)
  CALL BEST(N+1,1,1,0,DKK,-BB,F10)
  CALL BEST(N,2,2,3,DKK,-BB,F11)
  CALL BEST(N,0,0,1,DKK,-BB,F12)
  CALL BEST(N,2,2,1,DKK,-BB,F13)
  CALL BEST(N,1,1,2,DKK,-BB,F14)
  CALL BEST(N-1,0,0,3,DKK,-BB,F15)
  CALL BEST(N,1,2,3,DKK,-BB,F16)
  CALL BEST(N-1,1,1,2,DKK,-BB,F17)
  CALL BEST(N+1,0,0,3,DKK,-BB,F18)
  CALL BEST(N+1,1,1,2,DKK,-BB,F19)
  CALL BEST(N,0,0,3,DKK,-BB,F20)
  H1=-N*(2*N-1)*(-BB)**2.*AJ0*F1+N*(2*N-1)*(-BB)**2.*B1*F2/DY**2.-
& .5*(N-2)*(Y**2.-X**2.)*B2*F3+.5*N*(N+1)*(N-2)*AJ0*F4
  H1R=-N*(2*N-1)*(-BB)**2.*PAJ0*DKK*U3*F1-2.*N*(2*N-1)*U3*(-BB)**2.
& *B1*F2/DY**3.+N*(2*N-1)*(-BB)**2.*B1R*F2/DY**2.-(N-2)*(Y**2.-
& X**2.)*B2*F3/RAD(1)-.5*(N-2)*(Y**2.-X**2.)*B2R*F3+.5*N*(N+1)*(N-
& 2)*PAJ0*DKK*U3*F4
  H1S=-N*(2*N-1)*(-BB)**2.*PAJ0*DKK*RAD(1)*U2*F1-2.*N*(2*N-1)*U2*
& RAD(1)*(-BB)**2.*B1*F2/DY**3.+N*(2*N-1)*(-BB)**2.*B1S*F2/DY**2.
& -(N-2)*(Y**2.-X**2.)*B2*F3*Z/DY-.5*(N-2)*(Y**2.-X**2.)*B2S*F3
& +.5*N*(N+1)*(N-2)*DKK*RAD(1)*U2*F4*PAJ0
  H1F=N*(2*N-1)*(-BB)**2.*B1F*F2/DY**2.-2.*(N-2)*X*Y*B2*F3
  H2=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
& (N+1)*(N-2)*F4)*B1/DY**2.
  H2R=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
& (N+1)*(N-2)*F4)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H2S=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
& (N+1)*(N-2)*F4)*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H2F=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
& (N+1)*(N-2)*F4)*B1F/DY**2.
  H3=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*B1/DY**2.
  H3R=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*(B1R/
& DY**2.-2.*U3*B1/DY**3.)
  H3S=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*(B1S/
& DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H3F=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*B1F/
& DY**2.
  H4=.5*((Y**2.-X**2.)*B2*F7-N*(N+1)*AJ0*F8)
  H4R=.5*(2.*(Y**2.-X**2.)*B2*F7/RAD(1)+(Y**2.-X**2.)*B2R*F7-N*
& (N+1)*PAJ0*DKK*U3*F8)
  H4S=.5*(2.*Z*(Y**2.-X**2.)*B2*F7/DY+(Y**2.-X**2.)*B2S*F7-N*(N+1)
& *PAJ0*DKK*RAD(1)*U2*F8)
  H4F=2.*X*Y*B2*F7
  H5=-.5*((-BB)**2.*F9+N*(N+1)*F8)*B1/DY**2.
  H5R=-.5*((-BB)**2.*F9+N*(N+1)*F8)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H5S=-.5*((-BB)**2.*F9+N*(N+1)*F8)*(B1S/DY**2.-2.*RAD(1)*U2*B1/
& DY**3.)
```

```
  H5F=-.5*((-BB)**2.*F9+N*(N+1)*F8)*B1F/DY**2.
  H6=N*DKK*(-BB)**2.*B1*F10/DY**2.
  H6R=N*DKK*(-BB)**2.*F10*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H6S=N*DKK*(-BB)**2.*F10*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H6F=N*DKK*(-BB)**2.*F10*B1F/DY**2.
  H7=-.5*((Y**2.-X**2.)*B2*F11+N*(N+1)*AJ0*F12)
  H7R=-.5*(2.*(Y**2.-X**2.)*B2*F11/RAD(1)+(Y**2.-X**2.)*B2R*F11+N*
&(N+1)*PAJ0*DKK*U3*F12)
  H7S=-.5*(2.*(Y**2.-X**2.)*Z*B2*F11/DY+(Y**2.-X**2.)*B2S*F11+N*
&(N+1)*PAJ0*DKK*U2*RAD(1)*F12)
  H7F=-2.*X*Y*B2*F11
  H8=.5*((-BB)**2.*F13-N*(N+1)*F12)*B1/DY**2.
  H8R=.5*((-BB)**2.*F13-N*(N+1)*F12)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H8S=.5*((-BB)**2.*F13-N*(N+1)*F12)*(B1S/DY**2.-2.*U2*RAD(1)*B1/
&    DY**3.)
  H8F=.5*((-BB)**2.*F13-N*(N+1)*F12)*B1F/DY**2.
  H9=DKK*(-BB)**2.*F1*B1/DY**2.
  H9R=DKK*(-BB)**2.*F1*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H9S=DKK*(-BB)**2.*F1*(B1S/DY**2.-2.*U2*RAD(1)*B1/DY**3.)
  H9F=DKK*(-BB)**2.*F1*B1F/DY**2.
  H10=X*Y*B2*(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15
& /(-BB)**2.)
  H10R=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
& **2.)*(2.*X*Y*B2/RAD(1)+X*Y*B2R)
  H10S=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
& **2.)*(2.*Z*X*Y*B2/DY+X*Y*B2S)
  H10F=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
& **2.)*DY**2.*B2*DCOS(2.*FI)
  H11=X*Y*B2*(N*(2*N-1)*F16+(N-2)*F3)
  H11R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(N*(2*N-1)*F16+(N-2)*F3)
  H11S=(2.*Z*X*Y*B2/DY+X*Y*B2S)*(N*(2*N-1)*F16+(N-2)*F3)
  H11F=DY**2.*B2*DCOS(2.*FI)*(N*(2*N-1)*F16+(N-2)*F3)
  H12=DKK*X*Y*B2*(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)
  H12R=(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*(2.*X*Y*B2/RAD(1)
& +X*Y*B2R)*DKK
  H12S=(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*(2.*Z*X*Y*B2/DY
& +X*Y*B2S)*DKK
  H12F=DKK*(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*DY**2.*B2*
& DCOS(2.*FI)
  H13=.5*X*Y*B2*(F7-N*(N+1)*F18/(-BB)**2.)
  H13R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(F7-N*(N+1)*F18/(-BB)**2.)/2.
  H13S=(2.*X*Y*Z*B2/DY+X*Y*B2S)*(F7-N*(N+1)*F18/(-BB)**2.)/2.
  H13F=DY**2.*B2*DCOS(2.*FI)*(F7-N*(N+1)*F18/(-BB)**2.)/2.
  H14=-1.*X*Y*B2*F7
  H14R=-1.*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F7
  H14S=-1.*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F7
  H14F=-1.*DY**2.*B2*DCOS(2.*FI)*F7
  H15=N*DKK*X*Y*B2*F19
  H15R=N*DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F19
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```
  H15S=N*DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F19
  H15F=N*DKK*DY**2.*B2*DCOS(2.*FI)*F19
  H16=-.5*X*Y*B2*(F11+N*(N+1)*F20/(-BB)**2.)
  H16R=-.5*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16S=-.5*(2.*X*Y*Z*B2/DY+X*Y*B2S)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16F=-.5*DY**2.*B2*DCOS(2.*FI)*(F11+N*(N+1)*F20/(-BB)**2.)
  H17=X*Y*B2*F11
  H17R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F11
  H17S=(2.*X*Y*Z*B2/DY+X*Y*B2S)*F11
  H17F=DY**2.*B2*DCOS(2.*FI)*F11
  H18=DKK*X*Y*B2*F14
  H18R=DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F14
  H18S=DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F14
  H18F=DKK*DY**2.*B2*DCOS(2.*FI)*F14
  H19=-1.*X*AJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*
&F15/(-BB)**2.)/DKK**2./DY
  H19R=-1.*X*PAJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*
&F15/(-BB)**2.)/DKK/RAD(1)
  H19S=-1.*X*Z*PAJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*
&(N-2)*F15/(-BB)**2.)/DKK/DY
  H19F=Y*AJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*F15
&/(-BB)**2.)/DKK**2./DY
  H20=-1.*X*AJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DKK/DY
  H20R=-1.*X*PAJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/RAD(1)
  H20S=-1.*X*Z*PAJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DY
  H20F=Y*AJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DY/DKK
  H21=-.5*X*AJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DKK**2./DY
  H21R=-.5*X*PAJ1*(F7+N*(N+1)*F18/(-BB)**2.)/RAD(1)/DKK
  H21S=-.5*X*Z*PAJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DY/DKK
  H21F=.5*Y*AJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DY/DKK**2.
  H22=N*X*AJ1*F19/DKK/DY
  H22R=N*X*PAJ1*F19/RAD(1)
  H22S=N*X*Z*PAJ1*F19/DY
  H22F=-1.*N*Y*AJ1*F19/DY/DKK
  H23=.5*X*AJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DKK**2./DY
  H23R=.5*X*PAJ1*(F11-N*(N+1)*F20/(-BB)**2.)/RAD(1)/DKK
  H23S=.5*X*Z*PAJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DY/DKK
  H23F=-.5*Y*AJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DY/DKK**2.
  H24=X*AJ1*F14/DKK/DY
  H24R=X*PAJ1*F14/RAD(1)
  H24S=X*Z*PAJ1*F14/DY
  H24F=-1.*Y*AJ1*F14/DY/DKK
  ANN1(II)=WET(II)*(G5*H1+G6*H2+G1*H3)*DEXP(DKK)
  ANN1R(II)=WET(II)*(G5R*H1+G5*H1R+G6R*H2+G6*H2R+G1R*H3+G1*H3R)
&*DEXP(DKK)
  ANN1S(II)=WET(II)*(G5S*H1+G5*H1S+G6S*H2+G6*H2S+G1S*H3+G1*H3S)
&*DEXP(DKK)
  ANN1F(II)=WET(II)*(G5*H1F+G6*H2F+G1*H3F)*DEXP(DKK)
  BNN1(II)=WET(II)*(G5*H4+G6*H5+G1*H6)*DEXP(DKK)
```

```
      BNN1R(II)=WET(II)*(G5R*H4+G5*H4R+G6R*H5+G6*H5R+G1R*H6+G1*H6R)
     & *DEXP(DKK)
      BNN1S(II)=WET(II)*(G5S*H4+G5*H4S+G6S*H5+G6*H5S+G1S*H6+G1*H6S)
     & *DEXP(DKK)
      BNN1F(II)=WET(II)*(G5*H4F+G6*H5F+G1*H6F)*DEXP(DKK)
      CNN1(II)=WET(II)*(G5*H7+G6*H8+G1*H9)*DEXP(DKK)
      CNN1R(II)=WET(II)*(G5R*H7+G5*H7R+G6R*H8+G6*H8R+G1R*H9+G1*H9R)
     & *DEXP(DKK)
      CNN1S(II)=WET(II)*(G5S*H7+G5*H7S+G6S*H8+G6*H8S+G1S*H9+G1*H9S)
     & *DEXP(DKK)
      CNN1F(II)=WET(II)*(G5*H7F+G6*H8F+G1*H9F)*DEXP(DKK)
      ANN2(II)=WET(II)*(G6*H10+G3*H11+G1*H12)*DEXP(DKK)
      ANN2R(II)=WET(II)*(G6R*H10+G6*H10R+G3R*H11+G3*H11R+G1R*H12+G1*
     & H12R)*DEXP(DKK)
      ANN2S(II)=WET(II)*(G6S*H10+G6*H10S+G3S*H11+G3*H11S+G1S*H12+G1*
     & H12S)*DEXP(DKK)
      ANN2F(II)=WET(II)*(G6*H10F+G3*H11F+G1*H12F)*DEXP(DKK)
      BNN2(II)=WET(II)*(G6*H13+G3*H14+G1*H15)*DEXP(DKK)
      BNN2R(II)=WET(II)*(G6R*H13+G6*H13R+G3R*H14+G3*H14R+G1R*H15+G1*
     &H15R)*DEXP(DKK)
      BNN2S(II)=WET(II)*(G6S*H13+G6*H13S+G3S*H14+G3*H14S+G1S*H15+G1*
     &H15S)*DEXP(DKK)
      BNN2F(II)=WET(II)*(G6*H13F+G3*H14F+G1*H15F)*DEXP(DKK)
      CNN2(II)=WET(II)*(G6*H16+G3*H17+G1*H18)*DEXP(DKK)
      CNN2R(II)=WET(II)*(G6R*H16+G6*H16R+G3R*H17+G3*H17R+G1R*H18+G1*
     & H18R)*DEXP(DKK)
      CNN2S(II)=WET(II)*(G6S*H16+G6*H16S+G3S*H17+G3*H17S+G1S*H18+G1*
     & H18S)*DEXP(DKK)
      CNN2F(II)=WET(II)*(G6*H16F+G3*H17F+G1*H18F)*DEXP(DKK)
      ANN3(II)=WET(II)*(G2*H19+G4*H20)*DEXP(DKK)
      ANN3R(II)=WET(II)*(G2R*H19+G2*H19R+G4R*H20+G4*H20R)*DEXP(DKK)
      ANN3S(II)=WET(II)*(G2S*H19+G2*H19S+G4S*H20+G4*H20S)*DEXP(DKK)
      ANN3F(II)=WET(II)*(G2*H19F+G4*H20F)*DEXP(DKK)
      BNN3(II)=WET(II)*(G2*H21+G4*H22)*DEXP(DKK)
      BNN3R(II)=WET(II)*(G2R*H21+G2*H21R+G4R*H22+G4*H22R)*DEXP(DKK)
      BNN3S(II)=WET(II)*(G2S*H21+G2*H21S+G4S*H22+G4*H22S)*DEXP(DKK)
      BNN3F(II)=WET(II)*(G2*H21F+G4*H22F)*DEXP(DKK)
      CNN3(II)=WET(II)*(G2*H23+G4*H24)*DEXP(DKK)
      CNN3R(II)=WET(II)*(G2R*H23+G2*H23R+G4R*H24+G4*H24R)*DEXP(DKK)
      CNN3S(II)=WET(II)*(G2S*H23+G2*H23S+G4S*H24+G4*H24S)*DEXP(DKK)
      CNN3F(II)=WET(II)*(G2*H23F+G4*H24F)*DEXP(DKK)
2001  CONTINUE
      SUM1=0.D0
      SUM2=0.D0
      SUM3=0.D0
      SUM4=0.D0
      SUM5=0.D0
      SUM6=0.D0
      SUM7=0.D0
```

```
SUM8=0.D0
SUM9=0.D0
SUM10=0.D0
SUM11=0.D0
SUM12=0.D0
SUM13=0.D0
SUM14=0.D0
SUM15=0.D0
SUM16=0.D0
SUM17=0.D0
SUM18=0.D0
SUM19=0.D0
SUM20=0.D0
SUM21=0.D0
SUM22=0.D0
SUM23=0.D0
SUM24=0.D0
SUM25=0.D0
SUM26=0.D0
SUM27=0.D0
SUM28=0.D0
SUM29=0.D0
SUM30=0.D0
SUM31=0.D0
SUM32=0.D0
SUM33=0.D0
SUM34=0.D0
SUM35=0.D0
SUM36=0.D0
DO 1999 IJ=1,IN
SUM1=SUM1+ANN1(IJ)
SUM2=SUM2+ANN2(IJ)
SUM3=SUM3+ANN3(IJ)
SUM4=SUM4+BNN1(IJ)
SUM5=SUM5+BNN2(IJ)
SUM6=SUM6+BNN3(IJ)
SUM7=SUM7+CNN1(IJ)
SUM8=SUM8+CNN2(IJ)
SUM9=SUM9+CNN3(IJ)
SUM10=SUM10+ANN1R(IJ)
SUM11=SUM11+ANN2R(IJ)
SUM12=SUM12+ANN3R(IJ)
SUM13=SUM13+BNN1R(IJ)
SUM14=SUM14+BNN2R(IJ)
SUM15=SUM15+BNN3R(IJ)
SUM16=SUM16+CNN1R(IJ)
SUM17=SUM17+CNN2R(IJ)
SUM18=SUM18+CNN3R(IJ)
SUM19=SUM19+ANN1S(IJ)
```

```
      SUM20=SUM20+ANN2S(IJ)
      SUM21=SUM21+ANN3S(IJ)
      SUM22=SUM22+BNN1S(IJ)
      SUM23=SUM23+BNN2S(IJ)
      SUM24=SUM24+BNN3S(IJ)
      SUM25=SUM25+CNN1S(IJ)
      SUM26=SUM26+CNN2S(IJ)
      SUM27=SUM27+CNN3S(IJ)
      SUM28=SUM28+ANN1F(IJ)
      SUM29=SUM29+ANN2F(IJ)
      SUM30=SUM30+ANN3F(IJ)
      SUM31=SUM31+BNN1F(IJ)
      SUM32=SUM32+BNN2F(IJ)
      SUM33=SUM33+BNN3F(IJ)
      SUM34=SUM34+CNN1F(IJ)
      SUM35=SUM35+CNN2F(IJ)
      SUM36=SUM36+CNN3F(IJ)
1999  CONTINUE
      RETURN
      END

      SUBROUTINE BEST(N,M,J,L,ABK,ZZ1,BBB)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PI=DACOS(-1.D0)
      FFD=0.D0
      DO 104 IQ=0,INT(N/2)
      IF (N-2*IQ-M .LT. 0) THEN
      FFD1=0.D0
      GO TO 1435
      ELSE
      CALL GAMMA(N-2*IQ-M,AA1)
      CALL GAMMA(IQ,AA2)
      XZ=ABK*ABS(ZZ1)
      FFD1=((2/PI)**.5)/((-2.D0)**IQ)/AA2/AA1/(ZZ1)**(N+M)
       END IF
       CALL AKV(N,IQ,J,XZ,WK)
1435   CONTINUE
       FFD=FFD+FFD1*WK*(ABK*ABS(ZZ1))**(N-IQ+L-.5)
104    CONTINUE
       BBB=FFD
       IF (N .LT. M) THEN
       BBB=0.D0
       END IF
       RETURN
       END

       SUBROUTINE AKV(N,IQ,J,X,FDK)
       IMPLICIT DOUBLE PRECISION (A-H,O-Z)
       DIMENSION AAK(-20:80),FFK(-20:80)
```

```
      IF (N-IQ-J .GE. 1) THEN
      NN=N-IQ-J-1
      ELSE
      NN=N-IQ-J
      END IF
      PI=DACOS(-1.D0)
      AAK(0)=-1.*(.5D0*PI/X)/DEXP(X)
      AAK(1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      AAK(-1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(-2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(0)=(.5D0*PI/X)**.5/DEXP(X)
      FFK(1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(-1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(-2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      IF (IABS(NN) .LE. 2 ) THEN
      GO TO 2233
      END IF
      DO 502 I=3,IABS(NN)
      AAK(I)=AAK(I-2)-(2*I-1)*AAK(I-1)/X
      FFK(I)=AAK(I)/(-1.)**(I+1)/(.5*PI/X)**.5
      FFK(-I)=FFK(I)
502   CONTINUE
2233  CONTINUE
      FDK=FFK(NN)
4443  CONTINUE
      RETURN
      END

      SUBROUTINE GAMMA(J,AJK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IF (J .EQ. 0) THEN
      AJK=1.D0
      ELSE
      AJK=1.D0
      DO 300 I=1,J
      SS=DBLE(I)
      AJK=AJK*SS
300   CONTINUE
      END IF
      RETURN
      END

      SUBROUTINE BESSEL(CX,AJ,AJ0,AJ1,AJ2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      AJ0=0.D0
      AJ1=0.D0
      AJ2=0.D0
```

```
      DO 100 J=0,50
      CALL GAMMA(J,AJK)
      TJ=AJ0
      AJ0=AJ0+((-1.D0)**J)*(CX/2.)**(2*J)/(AJK)**2.
      IF (ABS(AJ0-TJ) .LE. 0.000000000000001 ) THEN
      GO TO    500
      END IF
100   CONTINUE
500   CONTINUE
      DO 107 J=0,50
      CALL GAMMA(J,AJK)
      TJ1=AJ1
      AJ1=AJ1+((-1.D0)**J)*(CX/2.)**(2*J+1)/((AJK)**2.)/(J+1)
      IF (ABS(AJ1-TJ1) .LE. 0.000000000000001 ) THEN
      GO TO 201
      END IF
107   CONTINUE
201   CONTINUE
      DO 108 J=0,50
      CALL GAMMA(J,AJK)
      TJ2=AJ2
      AJ2=AJ2+((-1.D0)**J)*(CX/2.)**(2*J+2)/((AJK)**2.)/(J+1)
     &/(J+2)
      IF (ABS(AJ2-TJ2)    .LE. 0.0000000000000001) THEN
      GO TO 200
      END IF
108   CONTINUE
200   CONTINUE
      AJ=-1.*AJ1
      RETURN
      END

      SUBROUTINE XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN(96),RAD(2),AN1(96),AN2(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=-1.*DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      CALL BEST(N+1,1,1,0,DKK,-BB,VV1)
      AN(II)=WET(II)*N*(-1.D0*(BB)**2.*DEXP(E3)*AJ1*VV1)*DEXP(DKK)
      AN1(II)=WET(II)*N*(DKK*U2*DEXP(E3)*(BB)**2.*AJ1*VV1-DKK
     &*DEXP(E3)*(BB)**2.*PAJ1*U3*VV1)*DEXP(DKK)
```

```
      AN2(II)=WET(II)*N*(-DKK*RAD(1)*U3*DEXP(E3)*(BB)**2.*VV1*AJ1
     &-DKK*RAD(1)*U2*DEXP(E3)*(BB)**2.*VV1*PAJ1)*DEXP(DKK)
2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN(IJ)
      SM2=SM2+AN1(IJ)
      SM3=SM3+AN2(IJ)
1999  CONTINUE
      RETURN
      END



CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C               FOR LINEAR TEMPERATURE PROFILE                 C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC



      SUBROUTINE XRD(N,BB,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN(96),RAD(2),AN1(96),AN2(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=-1.*DDK(II)*(ZZ+BB)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      CALL BEST(N,1,1,0,DKK,-BB,VV1)
      AN(II)=WET(II)*(-1.*DKK*(BB)**2.*DEXP(E3)*AJ1*VV1)*DEXP(DDK(II))
      AN1(II)=WET(II)*(DKK**2.*U2*DEXP(E3)*(BB)**2.*AJ1*VV1-DKK**2.
     & *DEXP(E3)*(BB)**2.*PAJ1*U3*VV1)*DEXP(DKK)
      AN2(II)=WET(II)*(-1.*DKK**2.*RAD(1)*U3*DEXP(E3)*(BB)**2.*VV1*AJ1
     & -DKK**2.*RAD(1)*U2*DEXP(E3)*(-BB)**2.*VV1*PAJ1)*DEXP(DKK)
2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      DO 1999 IJ=1,IN
```

```
      SM1=SM1+AN(IJ)
      SM2=SM2+AN1(IJ)
      SM3=SM3+AN2(IJ)
1999  CONTINUE
      RETURN
      END
```

Appendix E4-2: Computer programming source code for estimating the thermophoretic velocity of one spherical colloid parallel two insulated plates.

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(500,501),RAD(2),DDK(96),WET(96),B(500,501),BF(500,3)
      INTEGER T,GG,LL1,LL2,LBB,LCC,GGG
      OPEN (24,FILE='WET3.DAT',STATUS='OLD')
      OPEN (25,FILE='DDTTH1-0-0-10.DAT',STATUS='NEW')
      OPEN (23,FILE='GAUSS80.DAT',STATUS='OLD')
      IN=80
      TR=1.D0
      BB=0.1D0
      ETK=10.D0
      CC=BB*TR
      DO 1001 I=1,IN
      READ (23,*) DDK(I),WET(I)
1001  CONTINUE
      T=1
      PI=DACOS(-1.D0)
      FI=.01*PI/180.
      U4=DCOS(FI)
      U5=DSIN(FI)
      DO 3231    IUY=1,50
      READ (24,*) CV,NX
      RAD(1)=CV*BB
      CONST1=0.D0*RAD(1)
      CONST2=0.D0*RAD(1)
      GGG=2*NX
      DO 511 I=1,T
      DO 512 J=1,NX
      NU=J+NX*(I-1)
      NY=J+NX*(I-1)+T*NX
      DO 513 K=1,T
      CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      B(NU,GGG+1)=-1.*RAD(1)*U3+U3*CONST1
      B(NY,GGG+1)=-1.*U3
      DO 514 N=1,NX
      NZ=(2*N-1)+2*NX*(K-1)
      NL=2*N+2*NX*(K-1)
      CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      CALL XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      B(NU,NZ)=R2**(-N-1)*W1+SM1
     &-(SM2-(N+1)*R2**(-N-2)*W1)*CONST1
      B(NU,NL)=-R2**N*W1
      B(NY,NZ)=(-N-1)*R2**(-N-2)*W1+SM2
      B(NY,NL)=-ETK*N*R2**(N-1)*W1
```

```
514    CONTINUE
513    CONTINUE
512    CONTINUE
511    CONTINUE

       LL1=500
       LL2=501
       LBB=GGG
       LCC=GGG+1
       CALL GAUSL (LL1,LL2,LBB,LCC,B)
       GG=T*NX
       DO 7765 NN=1,3
       DO 111 I=1,T
       DO 112 J=1,NX
       NA=J+NX*(I-1)
       NB=J+NX*(I-1)+T*NX
       NC=J+NX*(I-1)+2*T*NX
       DO 113 K=1,T

       CALL FU(I,J,K,NX,RAD,PI,U2,U3,R2)
       IF (NN .EQ. 1) THEN
       A(NA,3*GG+1)=U3*U4
       A(NB,3*GG+1)=U2*U4
       A(NC,3*GG+1)=-1.*U5
       END IF

       IF(NN .EQ. 2) THEN
       A(NA,3*GG+1)=0.D0
       A(NB,3*GG+1)=U4
       A(NC,3*GG+1)=-1.*U2*U5
       END IF

       DO 114 N=1,NX
       NE=(3*N-2)+3*NX*(K-1)
       NG=(3*N-1)+3*NX*(K-1)
       NI=(3*N-0)+3*NX*(K-1)
       CALL FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
       CALL FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
       CALL FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
       CALL XXD(FI,N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,
      &WET,SUM1,SUM2,SUM3,
      &SUM4,SUM5,SUM6,SUM7,SUM8,SUM9,SUM10,
      &SUM11,SUM12,SUM13,SUM14,
      &SUM17,SUM18,SUM19,SUM20,SUM21,SUM22,
      &SUM23,SUM24,SUM25,SUM26,
      &SUM27,SUM28,SUM29,SUM30,SUM31,SUM32,
      &SUM33,SUM34,SUM35,SUM36,
      &SUM15,SUM16)
```

```
  AA1=((2.*N*(2*N-1)*U3*W1*U4**2.+(N-2)*WW2*DCOS(2.*FI)-N*(N+1)
&*(N-2)*WW)/2./R2**(N))
  BB1=-1.*(WWW2*DCOS(2.*FI)-N*(N+1)*WWW)/2./R2**(N+2)
  CC1=(W2*DCOS(2.*FI)+N*(N+1)*W)/2./R2**(N+1)
  AA2=(N*(2*N-1)*U3*W1+(N-2)*WW2)*U4*U5/R2**(N)
  BB2=-1.*(WWW2*U4*U5)/R2**(N+2)
  CC2=(W2*U4*U5)/R2**(N+1)
  AA3=(N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U4/R2**N
  BB3=-1.*(N*WWW1*U4)/R2**(N+2)
  CC3=-1.*(W1*U4)/R2**(N+1)
  AA1R=-1.*N*AA1/R2
  BB1R=-1.*(N+2)*BB1/R2
  CC1R=-1.*(N+1)*CC1/R2
  AA2R=-1.*N*AA2/R2
  BB2R=-1.*(N+2)*BB2/R2
  CC2R=-1.*(N+1)*CC2/R2
  AA3R=-1.*N*AA3/R2
  BB3R=-1.*(N+2)*BB3/R2
  CC3R=-1.*(N+1)*CC3/R2
  AA1S=(2.*N*(2*N-1)*U2*W1*U4**2.-2.*N*(2*N-1)*U3**2.*PW1*U4**2.-
&(N-2)*U3*PWW2*DCOS(2.*FI)+N*(N+1)*(N-2)*U3*PWW)/2./R2**N
  BB1S=-1.*(-1.*U3*PWWW2*DCOS(2.*FI)
&+N*(N+1)*U3*PWWW)/2./R2**(N+2)
  CC1S=(-1.*U3*PW2*DCOS(2.*FI)-U3*N*(N+1)*PW)/2./R2**(N+1)
  AA2S=(U2*N*(2*N-1)*W1-N*(2*N-1)*U3**2.*PW1-U3*(N-2)*PWW2)*U4*
&U5/R2**N
  BB2S=(U3*PWWW2*U4*U5)/R2**(N+2)
  CC2S=(-1.*U3*PW2*U4*U5)/R2**(N+1)
  AA3S=(-1.*N*(2.*N-1)*U3*W1-U2*U3*N*(2*N-1)*PW1+U3*(N+1)*(N-2)
&*PWW1)*U4/R2**N
  BB3S=U3*N*PWWW1*U4/R2**(N+2)
  CC3S=U3*PW1*U4/R2**(N+1)
  AA1F=((-2.*N*(2*N-1)*U3*W1*U4*U5-(N-2)*WW2*DSIN(2.*FI)
&)/R2**(N))
  BB1F=WWW2*DSIN(2.*FI)/R2**(N+2)
  CC1F=-1.*W2*DSIN(2.*FI)/R2**(N+1)
  AA2F=(N*(2*N-1)*U3*W1+(N-2)*WW2)*DCOS(2.*FI)/R2**(N)
  BB2F=-1.*(WWW2*DCOS(2.*FI))/R2**(N+2)
  CC2F=(W2*DCOS(2.*FI))/R2**(N+1)
  AA3F=-1.*(N*(2.*N-1)*U2*W1-(N+1)*(N-2)*WW1)*U5/R2**N
  BB3F=(N*WWW1*U5)/R2**(N+2)
  CC3F=(W1*U5)/R2**(N+1)
  A(NA,NE)=U3*U4*(AA1+SUM1)+U3*U5*(AA2+SUM2)+U2*(AA3+SUM3)
  A(NA,NG)=U3*U4*(BB1+SUM4)+U3*U5*(BB2+SUM5)+U2*(BB3+SUM6)
  A(NA,NI)=U3*U4*(CC1+SUM7)+U3*U5*(CC2+SUM8)+U2*(CC3+SUM9)
  A(NB,NE)=(U2*U4*(AA1+SUM1)+U2*U5*(AA2+SUM2)-U3*(AA3+SUM3))
&-CONST2*(U2*U4*(AA1R+SUM10)+U2*U5*(AA2R+SUM11)-
&U3*(AA3R+SUM12)
&+(U3*U4*(AA1S+SUM19)+U3*U5*(AA2S+SUM20)
```

```
     &+U2*(AA3S+SUM21))/R2)
      A(NB,NG)=(U2*U4*(BB1+SUM4)+U2*U5*(BB2+SUM5)-U3*(BB3+SUM6))
     &-CONST2*(U2*U4*(BB1R+SUM13)+U2*U5*(BB2R+SUM14)
     &-U3*(BB3R+SUM15)
     &+(U3*U4*(BB1S+SUM22)+U3*U5*(BB2S+SUM23)
     &+U2*(BB3S+SUM24))/R2)
      A(NB,NI)=(U2*U4*(CC1+SUM7)+U2*U5*(CC2+SUM8)-U3*(CC3+SUM9))
     &-CONST2*(U2*U4*(CC1R+SUM16)+U2*U5*(CC2R+SUM17)
     &-U3*(CC3R+SUM18)
     &+(U3*U4*(CC1S+SUM25)+U3*U5*(CC2S+SUM26)
     &+U2*(CC3S+SUM27))/R2)
      A(NC,NE)=(-1.*U5*(AA1+SUM1)+U4*(AA2+SUM2))
     &-CONST2*(-1.*U5*(AA1R+SUM10)
     &+U4*(AA2R+SUM11)+(U4*(AA1F+SUM28)+
     &U5*(AA2F+SUM29)+U2*(AA3F+SUM30)/U3)/R2)
      A(NC,NG)=(-1.*U5*(BB1+SUM4)+U4*(BB2+SUM5))
     &-CONST2*(-1.*U5*(BB1R+SUM13)+U4*(BB2R+SUM14)
     &+(U4*(BB1F+SUM31)+U5*(BB2F+SUM32)+U2*(BB3F+SUM33)/U3)/R2)
      A(NC,NI)=(-1.*U5*(CC1+SUM7)+U4*(CC2+SUM8))
     &-CONST2*(-1.*U5*(CC1R+SUM16)
     &+U4*(CC2R+SUM17)+(U4*(CC1F+SUM34)+
     &U5*(CC2F+SUM35)+U2*(CC3F+SUM36)/U3)/R2)
114   CONTINUE
113   CONTINUE
112   CONTINUE
111   CONTINUE

       IF (NN .EQ. 3) THEN
       DO 811 J=1,NX
       NA=J
       NB=J+NX
       NC=J+2*NX
       CALL FU(1,J,1,NX,RAD,PI,U2,U3,R2)
       VALUE=0.D0
       VALUE1=0.D0
       DO 713 KK=1,NX
       NZ=2*KK-1
       CALL FUCK2(U2,KK,W1,WW1,WWW1,PW1,PWW1,PWWW1)
       CALL XRD(KK,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
       VALUE=VALUE+B(NZ,GGG+1)*(R2**(-KK-1)*PW1*U4*(-1.*U3)+SM3)
       VALUE1=VALUE1+B(NZ,GGG+1)*(R2**(-KK-1)*W1*(-1.*U5)-U5*SM1)
713    CONTINUE
       A(NA,3*GG+1)=0.D0
       A(NB,3*GG+1)=(RAD(1)*U2*U4+VALUE)/RAD(1)
       A(NC,3*GG+1)=(-1.*RAD(1)*U3*U5+VALUE1)/RAD(1)/U3
811   CONTINUE
      END IF

      LL1=500
```

```
      LL2=501
      LBB=3*GG
      LCC=3*GG+1
      CALL GAUSL (LL1,LL2,LBB,LCC,A)
      DO 999 I=1,3*GG
      BF(I,NN)=A(I,3*GG+1)
999   CONTINUE
7765  CONTINUE
      VVU=-2*(1+ETK*CONST1/RAD(1))/
     &((1+2*CONST2/RAD(1))*(2+ETK+2*ETK*CONST1/RAD(1)))
      HGD=-1*(BF(1,3)*BF(3,2)-BF(1,2)*BF(3,3))/
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      HGR=-1*(BF(1,1)*BF(3,3)-BF(1,3)*BF(3,1))/
     &((BF(1,1)*BF(3,2)-BF(1,2)*BF(3,1))*VVU)
      WRITE (*,9)CV,HGD,HGR,XN
      WRITE (25,9)CV,HGD,HGR,XN
3231  CONTINUE
9     FORMAT (2(F12.5))
      STOP
      END

      SUBROUTINE FU(I,J,K,NX,RAD,PI,U2,U3,R2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION RAD(2)
      PID=1.D-3
      DTHETA=(PI-4.D0*PID)/(NX-2)
      IF(J==1) THEN
      Z=RAD(I)*DCOS(PID)
      V=RAD(I)*DSIN(PID)
      END IF
      IF((1<J) .AND. (J<=NX/2)) THEN
      Z=RAD(I)*DCOS(PID+(J-1)*DTHETA)
      V=RAD(I)*DSIN(PID+(J-1)*DTHETA)
      END IF
      IF(NX/2<J) THEN
      Z=RAD(I)*DCOS(PI/2.D0+(J-1-NX/2)*DTHETA)
      V=RAD(I)*DSIN(PI/2.D0+(J-1-NX/2)*DTHETA)
      END IF
      U2=Z/RAD(I)
      U3=V/RAD(I)
      R2=RAD(I)
      RETURN
      END

      SUBROUTINE GAUSL (N,M,II,JJ,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(N,M)
      DO 10 I=1,II
      AA=0.E0
```

```
      DO 9 J=1,II
9     AA=AA+ABS(A(I,J))
      DO 10 J=1,JJ
10    A(I,J)=A(I,J)/AA
      CALL XXXXX (N,M,II,JJ-II,A)
      RETURN
      END

      SUBROUTINE XXXXX (ND,NCOL,N,NS,A)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(ND,NCOL)
      N1=N+1
      NT=N+NS
      IF(N.EQ.1) GO TO 50
      DO 10 I=2,N
      IP=I-1
      I1=IP
      X=ABS(A(I1,I1))
      DO 11 J=I,N
      IF(ABS(A(J,I1)).LT.X) GO TO 11
      X=ABS(A(J,I1))
      IP=J
11    CONTINUE
      IF(IP.EQ.I1) GO TO 13
      DO 12 J=I1,NT
      X=A(I1,J)
      A(I1,J)=A(IP,J)
12    A(IP,J)=X
13    DO 10 J=I,N
      X=A(J,I1)/A(I1,I1)
      DO 10 K=I,NT
10    A(J,K)=A(J,K)-X*A(I1,K)
50    DO 20 IP=1,N
      I=N1-IP
      DO 20 K=N1,NT
      A(I,K)=A(I,K)/A(I,I)
      IF(I.EQ.1) GO TO 20
      I1=I-1
      DO 25 J=1,I1
25    A(J,K)=A(J,K)-A(I,K)*A(J,I)
20    CONTINUE
      RETURN
      END

      SUBROUTINE FUCK2(U2,N,W1,WW1,WWW1,PW1,PWW1,PWWW1)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PA(-1:600)
      PA(-1)=0.D0
      PA(0)=0.D0
```

```
      PA(1)=(1.-U2**2)**.5
      PA(2)=3.*U2*(1.-U2**2)**.5
      DO 100 J=1,N+1
      PA(J+1)=((2*J+1)*U2*PA(J)-(J+1)*PA(J-1))/(J)
100   CONTINUE
      W1=PA(N)
      WW1=PA(N-1)
      WWW1=PA(N+1)
      PW1=(N*U2*PA(N)-(N+1)*PA(N-1))/(U2**2.-1.)
      PWW1=((N-1)*U2*PA(N-1)-(N)*PA(N-2))/(U2**2.-1.)
      PWWW1=((N+1)*U2*PA(N+1)-(N+2)*PA(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK1(U2,N,W,WW,WWW,PW,PWW,PWWW)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PR(-1:600)
      PR(-1)=0.D0
      PR(0)=1.D0
      PR(1)=U2
      DO 34 I=2,N+1
      PR(I)=((2*I-1)*U2*PR(I-1)-(I-1)*PR(I-2))/I
34    CONTINUE
      W=PR(N)
      WW=PR(N-1)
      WWW=PR(N+1)
      PW=(N*U2*PR(N)-N*PR(N-1))/(U2**2.-1.)
      PWW=((N-1)*U2*PR(N-1)-(N-1)*PR(N-2))/(U2**2.-1.)
      PWWW=((N+1)*U2*PR(N+1)-(N+1)*PR(N))/(U2**2.-1.)
      RETURN
      END

      SUBROUTINE FUCK3(U2,N,W2,WW2,WWW2,PW2,PWW2,PWWW2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION PB(-1:600)
      PB(-1)=0.D0
      PB(0)=0.D0
      PB(1)=0.D0
      PB(2)=3.*(1.-U2**2)
      DO 150 K=2,N+1
      PB(K+1)=((2*K+1)*U2*PB(K)-(K+2)*PB(K-1))/(K-1)
150   CONTINUE
      W2=PB(N)
      WW2=PB(N-1)
      WWW2=PB(N+1)
      PW2=(N*U2*PB(N)-(N+2)*PB(N-1))/(U2**2.-1.)
      PWW2=((N-1)*U2*PB(N-1)-(N+1)*PB(N-2))/(U2**2.-1.)
      PWWW2=((N+1)*U2*PB(N+1)-(N+3)*PB(N))/(U2**2.-1.)
      RETURN
```

```
  END

  SUBROUTINE
&XXD(FI,N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SUM1,SUM2,
& SUM3,SUM4,SUM5,SUM6,SUM7,SUM8,
&SUM9,SUM10,SUM11,SUM12,SUM13,SUM14,
&SUM17,SUM18,SUM19,SUM20,SUM21,
&SUM22,SUM23,SUM24,SUM25,SUM26,
& SUM27,SUM28,SUM29,SUM30,SUM31,SUM32,
&SUM33,SUM34,SUM35,SUM36
&,SUM15,SUM16)
  IMPLICIT DOUBLE PRECISION (A-H,O-Z)
  DIMENSION WET(96),DDK(96),RAD(2)
  DIMENSION ANN1(96),ANN2(96),ANN3(96),
&BNN1(96),BNN2(96),BNN3(96)
  DIMENSION CNN1(96),CNN2(96),CNN3(96),
&ANN1R(96),ANN2R(96),ANN3R(96)
  DIMENSION BNN1R(96),BNN2R(96),BNN3R(96),CNN1R(96),CNN2R(96)
  DIMENSION CNN3R(96),ANN1S(96),ANN2S(96),ANN3S(96),BNN1S(96)
  DIMENSION BNN2S(96),BNN3S(96),CNN1S(96),CNN2S(96),CNN3S(96)
  DIMENSION ANN1F(96),ANN2F(96),ANN3F(96),BNN1F(96),BNN2F(96)
  DIMENSION BNN3F(96),CNN1F(96),CNN2F(96),CNN3F(96)
  DO 2001 II=1,IN
  Z=RAD(1)*U2
  X=RAD(1)*U3*U4
  Y=RAD(1)*U3*U5
  DKK=DDK(II)
  DY=RAD(1)*U3
  DDY=DKK*DY
  CALL BESSEL(DDY,AJ,AJ0,AJ1,AJ2)
  PAJ0=-1.*AJ1
  PAJ1=.5*(AJ0-AJ2)
  B1=AJ0*X**2.+(Y**2.-X**2.)*AJ1/DDY
  B2=(AJ0-2.*AJ1/DDY)/DDY**2.
  B1R=(X**2.*PAJ0*DDY+2.*X**2.*AJ0+(Y**2.-X**2.)*(AJ1+PAJ1*DDY)
&/DDY)/RAD(1)
  B1S=Z*(X**2.*PAJ0*DDY+2.*X**2.*AJ0+(Y**2.-X**2.)*(AJ1+PAJ1*DDY
&)/DDY)/DY
  B1F=-2.*X*Y*AJ0+4*X*Y*AJ1/DDY
  B2R=(6.*AJ1/DDY-2.*AJ0+DDY*PAJ0-2.*PAJ1)/RAD(1)/DDY**2.
  B2S=Z*(6.*AJ1/DDY-2.*AJ0+DDY*PAJ0-2.*PAJ1)/DDY**2./DY
  E3=DKK*(Z+BB)
  E2=DKK*(Z-CC)
  E1=DKK*(BB+CC)
  DEL1=2.*DSINH(E1)
  DEL2=4.*((DSINH(E1))**2.-E1**2.)
  G1=4.*E1*E2*E3*(DSINH(E3)/E3+DSINH(E1)*DSINH(E2)/E1/E2)/DEL2
  G2=4.*E1*E2*E3*(DSINH(E3)/E3-DSINH(E1)*DSINH(E2)/E1/E2)/DEL2
  D1=4.*E1*E3*E2*(DSINH(E2)/E2+DSINH(E1)*DSINH(E3)/E1/E3)/DEL2
```

```
  D2=4.*E1*E3*E2*(DSINH(E2)/E2-DSINH(E1)*DSINH(E3)/E1/E3)/DEL2
  G1R=4*E1*DKK*U2*(E2+E3)*(DSINH(E3)/E3
&+DSINH(E1)*DSINH(E2)/E2/E1)
&/DEL2+4.*E1*E2*E3*DKK*U2*(DCOSH(E3)/E3-DSINH(E3)/E3**2.+
&DSINH(E1)*DCOSH(E2)/E2/E1-DSINH(E1)*DSINH(E2)/E1/E2**2.)/DEL2
  G2R=4*E1*DKK*U2*(E2+E3)*(DSINH(E3)/E3
&-DSINH(E1)*DSINH(E2)/E2/E1)
&/DEL2+4.*E1*E2*E3*DKK*U2*(DCOSH(E3)/E3-DSINH(E3)/E3**2.-
&DSINH(E1)*DCOSH(E2)/E2/E1+DSINH(E1)*DSINH(E2)/E1/E2**2.)/DEL2
  D1R=4*E1*DKK*U2*(E2+E3)*(DSINH(E2)/E2
&+DSINH(E1)*DSINH(E3)/E3/E1)
&/DEL2+4.*E1*E2*E3*DKK*U2*(DCOSH(E2)/E2-DSINH(E2)/E2**2.+
&DSINH(E1)*DCOSH(E3)/E3/E1-DSINH(E1)*DSINH(E3)/E1/E3**2.)/DEL2
  D2R=4*E1*DKK*U2*(E2+E3)*(DSINH(E2)/E2
&-DSINH(E1)*DSINH(E3)/E3/E1)
&/DEL2+4.*E1*E2*E3*DKK*U2*(DCOSH(E2)/E2-DSINH(E2)/E2**2.-
&DSINH(E1)*DCOSH(E3)/E3/E1+DSINH(E1)*DSINH(E3)/E1/E3**2.)/DEL2
  G1S=-1.*RAD(1)*U3*G1R/U2
  G2S=-1.*RAD(1)*U3*G2R/U2
  D1S=-1.*RAD(1)*U3*D1R/U2
  D2S=-1.*RAD(1)*U3*D2R/U2
  G3=4.*E1*(E2*(DCOSH(E3)
&-DSINH(E1)*DSINH(E2)/E1/E2)+E3*(DSINH(E3)/
&E3-DSINH(E1)*DCOSH(E2)/E1))/DEL2
  G4=4.*E1*(E2*(DCOSH(E3)-DSINH(E1)*DSINH(E2)/E1/E2)
&-E3*(DSINH(E3)/
&E3-DSINH(E1)*DCOSH(E2)/E1))/DEL2
  D3=4.*E1*(E3*(DCOSH(E2)
&-DSINH(E1)*DSINH(E3)/E1/E3)+E2*(DSINH(E2)/
&E2-DSINH(E1)*DCOSH(E3)/E1))/DEL2
  D4=4.*E1*(E3*(DCOSH(E2)-DSINH(E1)*DSINH(E3)/E1/E3)-
&E2*(DSINH(E2)/
&E2-DSINH(E1)*DCOSH(E3)/E1))/DEL2
  G3R=4.*E1*DKK*U2*((DCOSH(E3)
&-DSINH(E1)*DSINH(E2)/E1/E2)+E2*(DSINH
&(E3)-DSINH(E1)*DCOSH(E2)/E1/E2+DSINH(E1)*DSINH(E2)/E1/E2**2.)+(
&DSINH(E3)/E3-DSINH(E1)*DCOSH(E2)/E1)
&+E3*(DCOSH(E3)/E3-DSINH(E3)/
&E3**2.-DSINH(E1)*DSINH(E2)/E1))/DEL2
  G4R=4.*E1*DKK*U2*((DCOSH(E3)
&-DSINH(E1)*DSINH(E2)/E1/E2)+E2*(DSINH
&(E3)-DSINH(E1)*DCOSH(E2)/E1/E2+DSINH(E1)*DSINH(E2)/E1/E2**2.)-(
&DSINH(E3)/E3-DSINH(E1)*DCOSH(E2)/E1)
&-E3*(DCOSH(E3)/E3-DSINH(E3)/
&E3**2.-DSINH(E1)*DSINH(E2)/E1))/DEL2
  D3R=4.*E1*DKK*U2*((DCOSH(E2)
&-DSINH(E1)*DSINH(E3)/E1/E3)+E3*(DSINH
&(E2)-DSINH(E1)*DCOSH(E3)/E1/E3+DSINH(E1)*DSINH(E3)/E1/E3**2.)+(
&DSINH(E2)/E2-DSINH(E1)*DCOSH(E3)/E1)
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&+E2*(DCOSH(E2)/E2-DSINH(E2)/
&E2**2.-DSINH(E1)*DSINH(E3)/E1))/DEL2
 D4R=4.*E1*DKK*U2*((DCOSH(E2)
&-DSINH(E1)*DSINH(E3)/E1/E3)+E3*(DSINH
&(E2)-DSINH(E1)*DCOSH(E3)/E1/E3+DSINH(E1)*DSINH(E3)/E1/E3**2.)-(
&DSINH(E2)/E2-DSINH(E1)*DCOSH(E3)/E1)
&-E2*(DCOSH(E2)/E2-DSINH(E2)/
&E2**2.-DSINH(E1)*DSINH(E3)/E1))/DEL2
 G3S=-1.*RAD(1)*U3*G3R/U2
 G4S=-1.*RAD(1)*U3*G4R/U2
 D3S=-1.*RAD(1)*U3*D3R/U2
 D4S=-1.*RAD(1)*U3*D4R/U2
 G5=-2.*DSINH(E2)/DEL1
 G5R=-2.*DKK*U2*DCOSH(E2)/DEL1
 G5S=2.*RAD(1)*DKK*U3*DCOSH(E2)/DEL1
 D5=-2.*DSINH(E3)/DEL1
 D5R=-2.*DKK*U2*DCOSH(E3)/DEL1
 D5S=2.*RAD(1)*DKK*U3*DCOSH(E3)/DEL1
 G6=8.*E1**2.*(E3*DSINH(E1)*(DSINH(E3)/E3
&-DSINH(E1)*DCOSH(E2)/E1)/
&E1+E2*(DSINH(E1)*DCOSH(E3)/E1-DSINH(E2)/E2))/DEL1/DEL2
 D6=8.*E1**2.*(E2*DSINH(E1)*(DSINH(E2)/E2
&-DSINH(E1)*DCOSH(E3)/E1)/
&E1+E3*(DSINH(E1)*DCOSH(E2)/E1-DSINH(E3)/E3))/DEL1/DEL2
 G6R=8.*E1**2.*DKK*U2*(DSINH(E1)*(DSINH(E3)/E3
&-DSINH(E1)*DCOSH(E2)
&/E1)/E1+E3*DSINH(E1)*(DCOSH(E3)/E3-DSINH(E3)/E3**2.-DSINH(E1)*
&DSINH(E2)/E1)/E1+(DSINH(E1)*DCOSH(E3)/E1
&-DSINH(E2)/E2)+E2*(DSINH(
&E1)*DSINH(E3)/E1-DCOSH(E2)/E2+DSINH(E2)/E2**2.))/DEL1/DEL2
 D6R=8.*E1**2.*DKK*U2*(DSINH(E1)*(DSINH(E2)/E2
&-DSINH(E1)*DCOSH(E3)
&/E1)/E1+E2*DSINH(E1)*(DCOSH(E2)/E2-DSINH(E2)/E2**2.-DSINH(E1)*
&DSINH(E3)/E1)/E1+(DSINH(E1)*DCOSH(E2)/E1
&-DSINH(E3)/E3)+E3*(DSINH(
&E1)*DSINH(E2)/E1-DCOSH(E3)/E3+DSINH(E3)/E3**2.))/DEL1/DEL2
 G6S=-1.*RAD(1)*U3*G6R/U2
 D6S=-1.*RAD(1)*U3*D6R/U2
 CALL BEST(N,1,1,0,DKK,-BB,F1)
 CALL BEST(N,1,2,1,DKK,-BB,F2)
 CALL BEST(N-1,2,2,3,DKK,-BB,F3)
 CALL BEST(N-1,0,0,1,DKK,-BB,F4)
 CALL BEST(N-1,2,2,1,DKK,-BB,F5)
 CALL BEST(N-1,1,1,0,DKK,-BB,F6)
 CALL BEST(N+1,2,2,3,DKK,-BB,F7)
 CALL BEST(N+1,0,0,1,DKK,-BB,F8)
 CALL BEST(N+1,2,2,1,DKK,-BB,F9)
 CALL BEST(N+1,1,1,0,DKK,-BB,F10)
 CALL BEST(N,2,2,3,DKK,-BB,F11)
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  CALL BEST(N,0,0,1,DKK,-BB,F12)
  CALL BEST(N,2,2,1,DKK,-BB,F13)
  CALL BEST(N,1,1,2,DKK,-BB,F14)
  CALL BEST(N-1,0,0,3,DKK,-BB,F15)
  CALL BEST(N,1,2,3,DKK,-BB,F16)
  CALL BEST(N-1,1,1,2,DKK,-BB,F17)
  CALL BEST(N+1,0,0,3,DKK,-BB,F18)
  CALL BEST(N+1,1,1,2,DKK,-BB,F19)
  CALL BEST(N,0,0,3,DKK,-BB,F20)
  CALL BEST(N,1,1,0,DKK,CC,T1)
  CALL BEST(N,1,2,1,DKK,CC,T2)
  CALL BEST(N-1,2,2,3,DKK,CC,T3)
  CALL BEST(N-1,0,0,1,DKK,CC,T4)
  CALL BEST(N-1,2,2,1,DKK,CC,T5)
  CALL BEST(N-1,1,1,0,DKK,CC,T6)
  CALL BEST(N+1,2,2,3,DKK,CC,T7)
  CALL BEST(N+1,0,0,1,DKK,CC,T8)
  CALL BEST(N+1,2,2,1,DKK,CC,T9)
  CALL BEST(N+1,1,1,0,DKK,CC,T10)
  CALL BEST(N,2,2,3,DKK,CC,T11)
  CALL BEST(N,0,0,1,DKK,CC,T12)
  CALL BEST(N,2,2,1,DKK,CC,T13)
  CALL BEST(N,1,1,2,DKK,CC,T14)
  CALL BEST(N-1,0,0,3,DKK,CC,T15)
  CALL BEST(N,1,2,3,DKK,CC,T16)
  CALL BEST(N-1,1,1,2,DKK,CC,T17)
  CALL BEST(N+1,0,0,3,DKK,CC,T18)
  CALL BEST(N+1,1,1,2,DKK,CC,T19)
  CALL BEST(N,0,0,3,DKK,CC,T20)
  H1=-N*(2*N-1)*(-BB)**2.*AJ0*F1+N*(2*N-1)*(-BB)**2.*B1*F2/DY**2.-
&.5*(N-2)*(Y**2.-X**2.)*B2*F3+.5*N*(N+1)*(N-2)*AJ0*F4
  H1C=-N*(2*N-1)*CC**2.*AJ0*T1+N*(2*N-1)*CC**2.*B1*T2/DY**2.-
&.5*(N-2)*(Y**2.-X**2.)*B2*T3+.5*N*(N+1)*(N-2)*AJ0*T4
  H1R=-N*(2*N-1)*(-BB)**2.*PAJ0*DKK*U3*F1-2.*N*(2*N-1)*U3*(-BB)**2.
&*B1*F2/DY**3.+N*(2*N-1)*(-BB)**2.*B1R*F2/DY**2.-(N-2)*(Y**2.-
&X**2.)*B2*F3/RAD(1)-.5*(N-2)*(Y**2.-X**2.)*B2R*F3+.5*N*(N+1)*(N-
&2)*PAJ0*DKK*U3*F4
  H1CR=-N*(2*N-1)*CC**2.*PAJ0*DKK*U3*T1-2.*N*(2*N-1)*U3*CC**2.
&*B1*T2/DY**3.+N*(2*N-1)*CC**2.*B1R*T2/DY**2.-(N-2)*(Y**2.-
&X**2.)*B2*T3/RAD(1)-.5*(N-2)*(Y**2.-X**2.)*B2R*T3+.5*N*(N+1)*(N-
&2)*PAJ0*DKK*U3*T4
  H1S=-N*(2*N-1)*(-BB)**2.*PAJ0*DKK*RAD(1)*U2*F1-2.*N*(2*N-1)*U2*
&RAD(1)*(-BB)**2.*B1*F2/DY**3.+N*(2*N-1)*(-BB)**2.*B1S*F2/DY**2.
&-(N-2)*(Y**2.-X**2.)*B2*F3*Z/DY-.5*(N-2)*(Y**2.-X**2.)*B2S*F3
&+.5*N*(N+1)*(N-2)*DKK*RAD(1)*U2*F4*PAJ0
  H1CS=-N*(2*N-1)*CC**2.*PAJ0*DKK*RAD(1)*U2*T1-2.*N*(2*N-1)*U2*
&RAD(1)*CC**2.*B1*T2/DY**3.+N*(2*N-1)*CC**2.*B1S*T2/DY**2.
&-(N-2)*(Y**2.-X**2.)*B2*T3*Z/DY-.5*(N-2)*(Y**2.-X**2.)*B2S*T3
&+.5*N*(N+1)*(N-2)*DKK*RAD(1)*U2*T4*PAJ0
```

```
  H1F=N*(2*N-1)*(-BB)**2.*B1F*F2/DY**2.-2.*(N-2)*X*Y*B2*F3
  H1CF=N*(2*N-1)*CC**2.*B1F*T2/DY**2.-2.*(N-2)*X*Y*B2*T3
  H2=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
&(N+1)*(N-2)*F4)*B1/DY**2.
  H2C=(-1.*N*(2*N-1)*CC**2.*(T1-T2)+.5*(N-2)*CC**2.*T5+.5*N*
&(N+1)*(N-2)*T4)*B1/DY**2.
  H2R=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
&(N+1)*(N-2)*F4)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H2CR=(-1.*N*(2*N-1)*CC**2.*(T1-T2)+.5*(N-2)*CC**2.*T5+.5*N*
&(N+1)*(N-2)*T4)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H2S=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
&(N+1)*(N-2)*F4)*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H2CS=(-1.*N*(2*N-1)*CC**2.*(T1-T2)+.5*(N-2)*CC**2.*T5+.5*N*
&(N+1)*(N-2)*T4)*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H2F=(-1.*N*(2*N-1)*(-BB)**2.*(F1-F2)+.5*(N-2)*(-BB)**2.*F5+.5*N*
&(N+1)*(N-2)*F4)*B1F/DY**2.
  H2CF=(-1.*N*(2*N-1)*CC**2.*(T1-T2)+.5*(N-2)*CC**2.*T5+.5*N*
&(N+1)*(N-2)*T4)*B1F/DY**2.
  H3=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*B1/DY**2.
  H3C=DKK*CC**2.*(-1.*N*(2*N-1)*CC*T1+(N+1)*(N-2)*T6)*B1/DY**2.
  H3R=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*(B1R/
&DY**2.-2.*U3*B1/DY**3.)
  H3CR=DKK*CC**2.*(-1.*N*(2*N-1)*CC*T1+(N+1)*(N-2)*T6)*(B1R/
&DY**2.-2.*U3*B1/DY**3.)
  H3S=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*(B1S/
&DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H3CS=DKK*CC**2.*(-1.*N*(2*N-1)*CC*T1+(N+1)*(N-2)*T6)*(B1S/
&DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H3F=DKK*(-BB)**2.*(-1.*N*(2*N-1)*(-BB)*F1+(N+1)*(N-2)*F6)*B1F/
&DY**2.
  H3CF=DKK*CC**2.*(-1.*N*(2*N-1)*CC*T1+(N+1)*(N-2)*T6)*B1F/
&DY**2.
  H4=.5*((Y**2.-X**2.)*B2*F7-N*(N+1)*AJ0*F8)
  H4C=.5*((Y**2.-X**2.)*B2*T7-N*(N+1)*AJ0*T8)
  H4R=.5*(2.*(Y**2.-X**2.)*B2*F7/RAD(1)+(Y**2.-X**2.)*B2R*F7-N*
&(N+1)*PAJ0*DKK*U3*F8)
  H4CR=.5*(2.*(Y**2.-X**2.)*B2*T7/RAD(1)+(Y**2.-X**2.)*B2R*T7-N*
&(N+1)*PAJ0*DKK*U3*T8)
  H4S=.5*(2.*Z*(Y**2.-X**2.)*B2*F7/DY+(Y**2.-X**2.)*B2S*F7-N*(N+1)
&*PAJ0*DKK*RAD(1)*U2*F8)
  H4CS=.5*(2.*Z*(Y**2.-X**2.)*B2*T7/DY+(Y**2.-X**2.)*B2S*T7-N*(N+1)
&*PAJ0*DKK*RAD(1)*U2*T8)
  H4F=2.*X*Y*B2*F7
  H4CF=2.*X*Y*B2*T7
  H5=-.5*((-BB)**2.*F9+N*(N+1)*F8)*B1/DY**2.
  H5C=-.5*(CC**2.*T9+N*(N+1)*T8)*B1/DY**2.
  H5R=-.5*((-BB)**2.*F9+N*(N+1)*F8)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H5CR=-.5*(CC**2.*T9+N*(N+1)*T8)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H5S=-.5*((-BB)**2.*F9+N*(N+1)*F8)*(B1S/DY**2.-2.*RAD(1)*U2*B1/
```

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&DY**3.)
  H5CS=-.5*(CC**2.*T9+N*(N+1)*T8)*(B1S/DY**2.-2.*RAD(1)*U2*B1/
&DY**3.)
  H5F=-.5*((-BB)**2.*F9+N*(N+1)*F8)*B1F/DY**2.
  H5CF=-.5*(CC**2.*T9+N*(N+1)*T8)*B1F/DY**2.
  H6=N*DKK*(-BB)**2.*B1*F10/DY**2.
  H6R=N*DKK*(-BB)**2.*F10*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H6S=N*DKK*(-BB)**2.*F10*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H6F=N*DKK*(-BB)**2.*F10*B1F/DY**2.
  H6C=N*DKK*CC**2.*B1*T10/DY**2.
  H6CR=N*DKK*CC**2.*T10*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H6CS=N*DKK*CC**2.*T10*(B1S/DY**2.-2.*RAD(1)*U2*B1/DY**3.)
  H6CF=N*DKK*CC**2.*T10*B1F/DY**2.
  H7=-.5*((Y**2.-X**2.)*B2*F11+N*(N+1)*AJ0*F12)
  H7R=-.5*(2.*(Y**2.-X**2.)*B2*F11/RAD(1)+(Y**2.-X**2.)*B2R*F11+N*
&(N+1)*PAJ0*DKK*U3*F12)
  H7S=-.5*(2.*(Y**2.-X**2.)*Z*B2*F11/DY+(Y**2.-X**2.)*B2S*F11+N*
&(N+1)*PAJ0*DKK*U2*RAD(1)*F12)
  H7F=-2.*X*Y*B2*F11
  H7C=-.5*((Y**2.-X**2.)*B2*T11+N*(N+1)*AJ0*T12)
  H7CR=-.5*(2.*(Y**2.-X**2.)*B2*T11/RAD(1)+(Y**2.-X**2.)*B2R*T11+N*
&(N+1)*PAJ0*DKK*U3*T12)
  H7CS=-.5*(2.*(Y**2.-X**2.)*Z*B2*T11/DY+(Y**2.-X**2.)*B2S*T11+N*
&(N+1)*PAJ0*DKK*U2*RAD(1)*T12)
  H7CF=-2.*X*Y*B2*T11
  H8=.5*((-BB)**2.*F13-N*(N+1)*F12)*B1/DY**2.
  H8R=.5*((-BB)**2.*F13-N*(N+1)*F12)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H8S=.5*((-BB)**2.*F13-N*(N+1)*F12)*(B1S/DY**2.-2.*U2*RAD(1)*B1/
&DY**3.)
  H8F=.5*((-BB)**2.*F13-N*(N+1)*F12)*B1F/DY**2.
  H8C=.5*(CC**2.*T13-N*(N+1)*T12)*B1/DY**2.
  H8CR=.5*(CC**2.*T13-N*(N+1)*T12)*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H8CS=.5*(CC**2.*T13-N*(N+1)*T12)*(B1S/DY**2.-2.*U2*RAD(1)*B1/
&DY**3.)
  H8CF=.5*(CC**2.*T13-N*(N+1)*T12)*B1F/DY**2.
  H9=DKK*(-BB)**2.*F1*B1/DY**2.
  H9R=DKK*(-BB)**2.*F1*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H9S=DKK*(-BB)**2.*F1*(B1S/DY**2.-2.*U2*RAD(1)*B1/DY**3.)
  H9F=DKK*(-BB)**2.*F1*B1F/DY**2.
  H9C=DKK*CC**2.*T1*B1/DY**2.
  H9CR=DKK*CC**2.*T1*(B1R/DY**2.-2.*U3*B1/DY**3.)
  H9CS=DKK*CC**2.*T1*(B1S/DY**2.-2.*U2*RAD(1)*B1/DY**3.)
  H9CF=DKK*CC**2.*T1*B1F/DY**2.
  H10=X*Y*B2*(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15
&/(-BB)**2.)
  H10R=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
&**2.)*(2.*X*Y*B2/RAD(1)+X*Y*B2R)
  H10S=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
&**2.)*(2.*Z*X*Y*B2/DY+X*Y*B2S)
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  H10F=(-1.*N*(2*N-1)*F14-.5*(N-2)*F3+.5*N*(N+1)*(N-2)*F15/(-BB)
&**2.)*DY**2.*B2*DCOS(2.*FI)
  H10C=X*Y*B2*(-1.*N*(2*N-1)*T14-.5*(N-2)*T3+.5*N*(N+1)*(N-2)*T15
&/CC**2.)
  H10CR=(-1.*N*(2*N-1)*T14-.5*(N-2)*T3+.5*N*(N+1)*(N-2)*T15/CC
&**2.)*(2.*X*Y*B2/RAD(1)+X*Y*B2R)
  H10CS=(-1.*N*(2*N-1)*T14-.5*(N-2)*T3+.5*N*(N+1)*(N-2)*T15/CC
&**2.)*(2.*Z*X*Y*B2/DY+X*Y*B2S)
  H10CF=(-1.*N*(2*N-1)*T14-.5*(N-2)*T3+.5*N*(N+1)*(N-2)*T15/CC
&**2.)*DY**2.*B2*DCOS(2.*FI)
  H11=X*Y*B2*(N*(2*N-1)*F16+(N-2)*F3)
  H11R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(N*(2*N-1)*F16+(N-2)*F3)
  H11S=(2.*Z*X*Y*B2/DY+X*Y*B2S)*(N*(2*N-1)*F16+(N-2)*F3)
  H11F=DY**2.*B2*DCOS(2.*FI)*(N*(2*N-1)*F16+(N-2)*F3)
  H11C=X*Y*B2*(N*(2*N-1)*T16+(N-2)*T3)
  H11CR=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(N*(2*N-1)*T16+(N-2)*T3)
  H11CS=(2.*Z*X*Y*B2/DY+X*Y*B2S)*(N*(2*N-1)*T16+(N-2)*T3)
  H11CF=DY**2.*B2*DCOS(2.*FI)*(N*(2*N-1)*T16+(N-2)*T3)
  H12=DKK*X*Y*B2*(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)
  H12R=(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*(2.*X*Y*B2/RAD(1)
&+X*Y*B2R)*DKK
  H12S=(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*(2.*Z*X*Y*B2/DY
&+X*Y*B2S)*DKK
  H12F=DKK*(-1.*N*(2*N-1)*(-BB)*F14+(N+1)*(N-2)*F17)*DY**2.*B2*
&DCOS(2.*FI)
  H12C=DKK*X*Y*B2*(-1.*N*(2*N-1)*CC*T14+(N+1)*(N-2)*T17)
  H12CR=(-1.*N*(2*N-1)*CC*T14+(N+1)*(N-2)*T17)*(2.*X*Y*B2/RAD(1)
&+X*Y*B2R)*DKK
  H12CS=(-1.*N*(2*N-1)*CC*T14+(N+1)*(N-2)*T17)*(2.*Z*X*Y*B2/DY
&+X*Y*B2S)*DKK
  H12CF=DKK*(-1.*N*(2*N-1)*CC*T14+(N+1)*(N-2)*T17)*DY**2.*B2*
&DCOS(2.*FI)
  H13=.5*X*Y*B2*(F7-N*(N+1)*F18/(-BB)**2.)
  H13R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(F7-N*(N+1)*F18/(-BB)**2.)
  H13S=(2.*X*Y*Z*B2/DY+X*Y*B2S)*(F7-N*(N+1)*F18/(-BB)**2.)
  H13F=DY**2.*B2*DCOS(2.*FI)*(F7-N*(N+1)*F18/(-BB)**2.)
  H13C=.5*X*Y*B2*(T7-N*(N+1)*T18/CC**2.)
  H13CR=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(T7-N*(N+1)*T18/CC**2.)
  H13CS=(2.*X*Y*Z*B2/DY+X*Y*B2S)*(T7-N*(N+1)*T18/CC**2.)
  H13CF=DY**2.*B2*DCOS(2.*FI)*(T7-N*(N+1)*T18/CC**2.)
  H14=-1.*X*Y*B2*F7
  H14R=-1.*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F7
  H14S=-1.*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F7
  H14F=-1.*DY**2.*B2*DCOS(2.*FI)*F7
  H14C=-1.*X*Y*B2*T7
  H14CR=-1.*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*T7
  H14CS=-1.*(2.*X*Y*Z*B2/DY+X*Y*B2S)*T7
  H14CF=-1.*DY**2.*B2*DCOS(2.*FI)*T7
  H15=N*DKK*X*Y*B2*F19
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  H15R=N*DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F19
  H15S=N*DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F19
  H15F=N*DKK*DY**2.*B2*DCOS(2.*FI)*F19
  H15C=N*DKK*X*Y*B2*T19
  H15CR=N*DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*T19
  H15CS=N*DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*T19
  H15CF=N*DKK*DY**2.*B2*DCOS(2.*FI)*T19
  H16=-.5*X*Y*B2*(F11+N*(N+1)*F20/(-BB)**2.)
  H16R=-.5*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16S=-.5*(2.*X*Y*Z*B2/DY+X*Y*B2S)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16F=-.5*DY**2.*B2*DCOS(2.*FI)*(F11+N*(N+1)*F20/(-BB)**2.)
  H16C=-.5*X*Y*B2*(T11+N*(N+1)*T20/CC**2.)
  H16CR=-.5*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*(T11+N*(N+1)*T20/CC**2.)
  H16CS=-.5*(2.*X*Y*Z*B2/DY+X*Y*B2S)*(T11+N*(N+1)*T20/CC**2.)
  H16CF=-.5*DY**2.*B2*DCOS(2.*FI)*(T11+N*(N+1)*T20/CC**2.)
  H17=X*Y*B2*F11
  H17R=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F11
  H17S=(2.*X*Y*Z*B2/DY+X*Y*B2S)*F11
  H17F=DY**2.*B2*DCOS(2.*FI)*F11
  H17C=X*Y*B2*T11
  H17CR=(2.*X*Y*B2/RAD(1)+X*Y*B2R)*T11
  H17CS=(2.*X*Y*Z*B2/DY+X*Y*B2S)*T11
  H17CF=DY**2.*B2*DCOS(2.*FI)*T11
  H18=DKK*X*Y*B2*F14
  H18R=DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*F14
  H18S=DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*F14
  H18F=DKK*DY**2.*B2*DCOS(2.*FI)*F14
  H18C=DKK*X*Y*B2*T14
  H18CR=DKK*(2.*X*Y*B2/RAD(1)+X*Y*B2R)*T14
  H18CS=DKK*(2.*X*Y*Z*B2/DY+X*Y*B2S)*T14
  H18CF=DKK*DY**2.*B2*DCOS(2.*FI)*T14
  H19=-1.*X*AJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*
&F15/(-BB)**2.)/DKK**2./DY
  H19R=-1.*X*PAJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*
&F15/(-BB)**2.)/DKK/RAD(1)
  H19S=-1.*X*Z*PAJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*
&(N-2)*F15/(-BB)**2.)/DKK/DY
  H19F=Y*AJ1*(N*(2*N-1)*(F14-F16)-.5*(N-2)*F3-.5*N*(N+1)*(N-2)*F15
&/(-BB)**2.)/DKK**2./DY
  H19C=-1.*X*AJ1*(N*(2*N-1)*(T14-T16)-.5*(N-2)*T3-.5*N*(N+1)*(N-2)*
&T15/CC**2.)/DKK**2./DY
  H19CR=-1.*X*PAJ1*(N*(2*N-1)*(T14-T16)-.5*(N-2)*T3-.5*N*(N+1)*(N-2)
&*T15/CC**2.)/DKK/RAD(1)
  H19CS=-1.*X*Z*PAJ1*(N*(2*N-1)*(T14-T16)-.5*(N-2)*T3-.5*N*(N+1)*
&(N-2)*T15/CC**2.)/DKK/DY
  H19CF=Y*AJ1*(N*(2*N-1)*(T14-T16)-.5*(N-2)*T3-.5*N*(N+1)*(N-2)*T15
&/CC**2.)/DKK**2./DY
  H20=-1.*X*AJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DKK/DY
  H20R=-1.*X*PAJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/RAD(1)
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  H20S=-1.*X*Z*PAJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DY
  H20F=Y*AJ1*(N*(2*N-1)*(-BB)*F14-(N+1)*(N-2)*F17)/DY/DKK
  H20C=-1.*X*AJ1*(N*(2*N-1)*CC*T14-(N+1)*(N-2)*T17)/DKK/DY
  H20CR=-1.*X*PAJ1*(N*(2*N-1)*CC*T14-(N+1)*(N-2)*T17)/RAD(1)
  H20CS=-1.*X*Z*PAJ1*(N*(2*N-1)*CC*T14-(N+1)*(N-2)*T17)/DY
  H20CF=Y*AJ1*(N*(2*N-1)*CC*T14-(N+1)*(N-2)*T17)/DY/DKK
  H21=-.5*X*AJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DKK**2./DY
  H21R=-.5*X*PAJ1*(F7+N*(N+1)*F18/(-BB)**2.)/RAD(1)/DKK
  H21S=-.5*X*Z*PAJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DY/DKK
  H21F=.5*Y*AJ1*(F7+N*(N+1)*F18/(-BB)**2.)/DY/DKK**2.
  H21C=-.5*X*AJ1*(T7+N*(N+1)*T18/CC**2.)/DKK**2./DY
  H21CR=-.5*X*PAJ1*(T7+N*(N+1)*T18/CC**2.)/RAD(1)/DKK
  H21CS=-.5*X*Z*PAJ1*(T7+N*(N+1)*T18/CC**2.)/DY/DKK
  H21CF=.5*Y*AJ1*(T7+N*(N+1)*T18/CC**2.)/DY/DKK**2.
  H22=N*X*AJ1*F19/DKK/DY
  H22R=N*X*PAJ1*F19/RAD(1)
  H22S=N*X*Z*PAJ1*F19/DY
  H22F=-1.*N*Y*AJ1*F19/DY/DKK
  H22C=N*X*AJ1*T19/DKK/DY
  H22CR=N*X*PAJ1*T19/RAD(1)
  H22CS=N*X*Z*PAJ1*T19/DY
  H22CF=-1.*N*Y*AJ1*T19/DY/DKK
  H23=.5*X*AJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DKK**2./DY
  H23R=.5*X*PAJ1*(F11-N*(N+1)*F20/(-BB)**2.)/RAD(1)/DKK
  H23S=.5*X*Z*PAJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DY/DKK
  H23F=-.5*Y*AJ1*(F11-N*(N+1)*F20/(-BB)**2.)/DY/DKK**2.
  H23C=.5*X*AJ1*(T11-N*(N+1)*T20/CC**2.)/DKK**2./DY
  H23CR=.5*X*PAJ1*(T11-N*(N+1)*T20/CC**2.)/RAD(1)/DKK
  H23CS=.5*X*Z*PAJ1*(T11-N*(N+1)*T20/CC**2.)/DY/DKK
  H23CF=-.5*Y*AJ1*(T11-N*(N+1)*T20/CC**2.)/DY/DKK**2.
  H24=X*AJ1*F14/DKK/DY
  H24R=X*PAJ1*F14/RAD(1)
  H24S=X*Z*PAJ1*F14/DY
  H24F=-1.*Y*AJ1*F14/DY/DKK
  H24C=X*AJ1*T14/DKK/DY
  H24CR=X*PAJ1*T14/RAD(1)
  H24CS=X*Z*PAJ1*T14/DY
  H24CF=-1.*Y*AJ1*T14/DY/DKK
  ANN1(II)=WET(II)*(G5*H1+G6*H2+G1*H3-D5*H1C-D6*H2C-D1*H3C)*
&DEXP(DKK)
  ANN1R(II)=WET(II)*(G5R*H1+G5*H1R+G6R*H2+G6*H2R
&+G1R*H3+G1*H3R
&-D5R*H1C-D5*H1CR-D6R*H2C-D6*H2CR-D1R*H3C-D1*H3CR)
&*DEXP(DKK)
  ANN1S(II)=WET(II)*(G5S*H1+G5*H1S+G6S*H2
&+G6*H2S+G1S*H3+G1*H3S
&-D5S*H1C-D5*H1CS-D6S*H2C-D6*H2CS-D1S*H3C-D1*H3CS)
&*DEXP(DKK)
  ANN1F(II)=WET(II)*(G5*H1F+G6*H2F+G1*H3F
```

```
&-D5*H1CF-D6*H2CF-D1*H3CF)*DEXP(DKK)
  BNN1(II)=WET(II)*(G5*H4+G6*H5+G1*H6-
&D5*H4C-D6*H5C-D1*H6C)*DEXP(DKK)
  BNN1R(II)=WET(II)*(G5R*H4+G5*H4R+G6R*H5
&+G6*H5R+G1R*H6+G1*H6R
&-D5R*H4C-D5*H4CR-D6R*H5C-D6*H5CR-D1R*H6C-D1*H6CR)
&*DEXP(DKK)
  BNN1S(II)=WET(II)*(G5S*H4+G5*H4S+G6S*H5
&+G6*H5S+G1S*H6+G1*H6S
&-D5S*H4C-D5*H4CS-D6S*H5C-D6*H5CS-D1S*H6C-D1*H6CS)
&*DEXP(DKK)
  BNN1F(II)=WET(II)*(G5*H4F+G6*H5F+G1*H6F-
&D5*H4CF-D6*H5CF-D1*H6CF)*DEXP(DKK)
  CNN1(II)=WET(II)*(G5*H7+G6*H8+G1*H9-
&D5*H7C-D6*H8C-D1*H9C)*DEXP(DKK)
  CNN1R(II)=WET(II)*(G5R*H7+G5*H7R+G6R*H8
&+G6*H8R+G1R*H9+G1*H9R
&-D5R*H7C-D5*H7CR-D6R*H8C-D6*H8CR-D1R*H9C-D1*H9CR)
&*DEXP(DKK)
  CNN1S(II)=WET(II)*(G5S*H7+G5*H7S+G6S*H8
&+G6*H8S+G1S*H9+G1*H9S
&-D5S*H7C-D5*H7CS-D6S*H8C-D6*H8CS-D1S*H9C-D1*H9CS)
&*DEXP(DKK)
  CNN1F(II)=WET(II)*(G5*H7F+G6*H8F+G1*H9F-
&D5*H7CF-D6*H8CF-D1*H9CF)*DEXP(DKK)
  ANN2(II)=WET(II)*(G6*H10+G3*H11+G1*H12-
& D6*H10C-D3*H11C-D1*H12C)*DEXP(DKK)
  ANN2R(II)=WET(II)*(G6R*H10+G6*H10R+G3R*H11
&+G3*H11R+G1R*H12+G1*
&H12R-D6R*H10C-D6*H10CR-D3R*H11C-D3*H11CR-D1R*H12C-D1*
&H12CR)*DEXP(DKK)
  ANN2S(II)=WET(II)*(G6S*H10+G6*H10S+G3S*H11
&+G3*H11S+G1S*H12+G1*
&H12S-D6S*H10C-D6*H10CS-D3S*H11C-D3*H11CS-D1S*H12C-D1*
&H12CS)*DEXP(DKK)
  ANN2F(II)=WET(II)*(G6*H10F+G3*H11F+G1*H12F-
&D6*H10CF-D3*H11CF-D1*H12CF)*DEXP(DKK)
  BNN2(II)=WET(II)*(G6*H13+G3*H14+G1*H15-
&D6*H13C-D3*H14C-D1*H15C)*DEXP(DKK)
  BNN2R(II)=WET(II)*(G6R*H13+G6*H13R+G3R*H14
&+G3*H14R+G1R*H15+G1*
&H15R-D6R*H13C-D6*H13CR-D3R*H14C-D3*H14CR-D1R*H15C-D1*
&H15CR)*DEXP(DKK)
  BNN2S(II)=WET(II)*(G6S*H13+G6*H13S+G3S*H14
&+G3*H14S+G1S*H15+G1*
&H15S-D6S*H13C-D6*H13CS-D3S*H14C-D3*H14CS-D1S*H15C-D1*
&H15CS)*DEXP(DKK)
  BNN2F(II)=WET(II)*(G6*H13F+G3*H14F+G1*H15F-
&D6*H13CF-D3*H14CF-D1*H15CF)*DEXP(DKK)
```

```
      CNN2(II)=WET(II)*(G6*H16+G3*H17+G1*H18-
     &D6*H16C-D3*H17C-D1*H18C)*DEXP(DKK)
      CNN2R(II)=WET(II)*(G6R*H16+G6*H16R+G3R*H17
     &+G3*H17R+G1R*H18+G1*
     &H18R-D6R*H16C-D6*H16CR-D3R*H17C-D3*H17CR-D1R*H18C-D1*
     &H18CR)*DEXP(DKK)
      CNN2S(II)=WET(II)*(G6S*H16+G6*H16S+G3S*H17
     &+G3*H17S+G1S*H18+G1*
     &H18S-D6S*H16C-D6*H16CS-D3S*H17C-D3*H17CS-D1S*H18C-D1*
     &H18CS)*DEXP(DKK)
      CNN2F(II)=WET(II)*(G6*H16F+G3*H17F+G1*H18F-
     &D6*H16CF-D3*H17CF-D1*H18CF)*DEXP(DKK)
      ANN3(II)=WET(II)*(G2*H19+G4*H20-D2*H19C-D4*H20C)*DEXP(DKK)
      ANN3R(II)=WET(II)*(G2R*H19+G2*H19R+G4R*H20+G4*H20R-
     &D2R*H19C-D2*H19CR-D4R*H20C-D4*H20CR)*DEXP(DKK)
      ANN3S(II)=WET(II)*(G2S*H19+G2*H19S+G4S*H20+G4*H20S-
     &D2S*H19C-D2*H19CS-D4S*H20C-D4*H20CS)*DEXP(DKK)
      ANN3F(II)=WET(II)*(G2*H19F+G4*H20F-D2*H19CF
     &-D4*H20CF)*DEXP(DKK)
      BNN3(II)=WET(II)*(G2*H21+G4*H22-D2*H21C-D4*H22C)*DEXP(DKK)
      BNN3R(II)=WET(II)*(G2R*H21+G2*H21R+G4R*H22+G4*H22R-
     &D2R*H21C-D2*H21CR-D4R*H22C-D4*H22CR)*DEXP(DKK)
      BNN3S(II)=WET(II)*(G2S*H21+G2*H21S+G4S*H22+G4*H22S-
     &D2S*H21C-D2*H21CS-D4S*H22C-D4*H22CS)*DEXP(DKK)
      BNN3F(II)=WET(II)*(G2*H21F+G4*H22F-D2*H21CF-
     &D4*H22CF)*DEXP(DKK)
      CNN3(II)=WET(II)*(G2*H23+G4*H24-D2*H23C-D4*H24C)*DEXP(DKK)
      CNN3R(II)=WET(II)*(G2R*H23+G2*H23R+G4R*H24+G4*H24R-
     &D2R*H23C-D2*H23CR-D4R*H24C-D4*H24CR)*DEXP(DKK)
      CNN3S(II)=WET(II)*(G2S*H23+G2*H23S+G4S*H24+G4*H24S-
     &D2S*H23C-D2*H23CS-D4S*H24C-D4*H24CS)*DEXP(DKK)
      CNN3F(II)=WET(II)*(G2*H23F+G4*H24F-D2*H23CF
     &-D4*H24CF)*DEXP(DKK)
 2001 CONTINUE
      SUM1=0.D0
      SUM2=0.D0
      SUM3=0.D0
      SUM4=0.D0
      SUM5=0.D0
      SUM6=0.D0
      SUM7=0.D0
      SUM8=0.D0
      SUM9=0.D0
      SUM10=0.D0
      SUM11=0.D0
      SUM12=0.D0
      SUM13=0.D0
      SUM14=0.D0
      SUM15=0.D0
```

```
SUM16=0.D0
SUM17=0.D0
SUM18=0.D0
SUM19=0.D0
SUM20=0.D0
SUM21=0.D0
SUM22=0.D0
SUM23=0.D0
SUM24=0.D0
SUM25=0.D0
SUM26=0.D0
SUM27=0.D0
SUM28=0.D0
SUM29=0.D0
SUM30=0.D0
SUM31=0.D0
SUM32=0.D0
SUM33=0.D0
SUM34=0.D0
SUM35=0.D0
SUM36=0.D0
DO 1999 IJ=1,IN
SUM1=SUM1+ANN1(IJ)
SUM2=SUM2+ANN2(IJ)
SUM3=SUM3+ANN3(IJ)
SUM4=SUM4+BNN1(IJ)
SUM5=SUM5+BNN2(IJ)
SUM6=SUM6+BNN3(IJ)
SUM7=SUM7+CNN1(IJ)
SUM8=SUM8+CNN2(IJ)
SUM9=SUM9+CNN3(IJ)
SUM10=SUM10+ANN1R(IJ)
SUM11=SUM11+ANN2R(IJ)
SUM12=SUM12+ANN3R(IJ)
SUM13=SUM13+BNN1R(IJ)
SUM14=SUM14+BNN2R(IJ)
SUM15=SUM15+BNN3R(IJ)
SUM16=SUM16+CNN1R(IJ)
SUM17=SUM17+CNN2R(IJ)
SUM18=SUM18+CNN3R(IJ)
SUM19=SUM19+ANN1S(IJ)
SUM20=SUM20+ANN2S(IJ)
SUM21=SUM21+ANN3S(IJ)
SUM22=SUM22+BNN1S(IJ)
SUM23=SUM23+BNN2S(IJ)
SUM24=SUM24+BNN3S(IJ)
SUM25=SUM25+CNN1S(IJ)
SUM26=SUM26+CNN2S(IJ)
SUM27=SUM27+CNN3S(IJ)
```

```
      SUM28=SUM28+ANN1F(IJ)
      SUM29=SUM29+ANN2F(IJ)
      SUM30=SUM30+ANN3F(IJ)
      SUM31=SUM31+BNN1F(IJ)
      SUM32=SUM32+BNN2F(IJ)
      SUM33=SUM33+BNN3F(IJ)
      SUM34=SUM34+CNN1F(IJ)
      SUM35=SUM35+CNN2F(IJ)
      SUM36=SUM36+CNN3F(IJ)
1999  CONTINUE
      RETURN
      END

      SUBROUTINE BEST(N,M,J,L,ABK,ZZ1,BBB)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PI=DACOS(-1.D0)
      FFD=0.D0
      DO 104 IQ=0,INT(N/2)
      IF (N-2*IQ-M .LT. 0) THEN
      FFD1=0.D0
      GO TO 1435
      ELSE
      CALL GAMMA(N-2*IQ-M,AA1)
      CALL GAMMA(IQ,AA2)
      XZ=ABK*ABS(ZZ1)
      FFD1=((2/PI)**.5)/((-2.D0)**IQ)/AA2/AA1/(ZZ1)**(N+M)
      END IF
      CALL AKV(N,IQ,J,XZ,WK)
1435  CONTINUE
      FFD=FFD+FFD1*WK*(ABK*ABS(ZZ1))**(N-IQ+L-.5)
104   CONTINUE
      BBB=FFD
      IF (N .LT. M) THEN
      BBB=0.D0
      END IF
      RETURN
      END
      SUBROUTINE AKV(N,IQ,J,X,FDK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION AAK(-20:80),FFK(-20:80)
      IF (N-IQ-J .GE. 1) THEN
      NN=N-IQ-J-1
      ELSE
      NN=N-IQ-J
      END IF
      PI=DACOS(-1.D0)
      AAK(0)=-1.*(.5D0*PI/X)/DEXP(X)
      AAK(1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
```

```
      AAK(-1)=(.5D0*PI/X)*(1+1/X)/DEXP(X)
      AAK(-2)=-1.*(.5D0*PI/X)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(0)=(.5D0*PI/X)**.5/DEXP(X)
      FFK(1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      FFK(-1)=((.5D0*PI/X)**.5)*(1+1/X)/DEXP(X)
      FFK(-2)=((.5D0*PI/X)**.5)*(1+3./X+3./X**2.)/DEXP(X)
      IF (IABS(NN) .LE. 2 ) THEN
      GO TO 2233
      END IF
      DO 502 I=3,IABS(NN)
      AAK(I)=AAK(I-2)-(2*I-1)*AAK(I-1)/X
      FFK(I)=AAK(I)/(-1.)**(I+1)/(.5*PI/X)**.5
      FFK(-I)=FFK(I)
502   CONTINUE
2233  CONTINUE
      FDK=FFK(NN)
4443  CONTINUE
      RETURN
      END

      SUBROUTINE GAMMA(J,AJK)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IF (J .EQ. 0) THEN
      AJK=1.D0
      ELSE
      AJK=1.D0
      DO 300 I=1,J
      SS=DBLE(I)
      AJK=AJK*SS
300   CONTINUE
      END IF
      RETURN
      END

      SUBROUTINE BESSEL(CX,AJ,AJ0,AJ1,AJ2)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      AJ0=0.D0
      AJ1=0.D0
      AJ2=0.D0
      DO 100 J=0,50
      CALL GAMMA(J,AJK)
      TJ=AJ0
      AJ0=AJ0+((-1.D0)**J)*(CX/2.)**(2*J)/(AJK)**2.
      IF (ABS(AJ0-TJ) .LE. 0.000000000000001 ) THEN
      GO TO    500
      END IF
100   CONTINUE
500   CONTINUE
```

```
      DO 107 J=0,50
      CALL GAMMA(J,AJK)
      TJ1=AJ1
      AJ1=AJ1+((-1.D0)**J)*(CX/2.)**(2*J+1)/((AJK)**2.)/(J+1)
      IF (ABS(AJ1-TJ1) .LE. 0.000000000000001 ) THEN
      GO TO 201
      END IF
107   CONTINUE
201   CONTINUE
      DO 108 J=0,50
      CALL GAMMA(J,AJK)
      TJ2=AJ2
      AJ2=AJ2+((-1.D0)**J)*(CX/2.)**(2*J+2)/((AJK)**2.)/(J+1)
     &/(J+2)
      IF (ABS(AJ2-TJ2)    .LE. 0.0000000000000001) THEN
      GO TO 200
      END IF
108   CONTINUE
200   CONTINUE
      AJ=-1.*AJ1
      RETURN
      END

      SUBROUTINE XRD(N,BB,CC,IN,RAD,U2,U3,
     &U4,U5,DDK,WET,SM1,SM2,SM3)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN(96),RAD(2),AN1(96),AN2(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      E2=DDK(II)*(ZZ-CC)
      E1=DDK(II)*(BB+CC)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)
      CALL BEST(N+1,1,1,0,DKK,-BB,VV1)
      CALL BEST (N+1,1,1,0,DKK,CC,VV2)
      AN(II)=WET(II)*N*((CC)**2.*DCOSH(E3)*AJ1*VV2/DSINH(E1)-
     &(-BB)**2.*AJ1*VV1*DCOSH(E2)/DSINH(E1))*DEXP(DKK)
      AN1(II)=WET(II)*N*(DKK*CC**2.*U2*DSINH(E3)*AJ1*U4*VV2/DSINH(
     &E1)+DKK*CC**2.*U3*DCOSH(E3)*PAJ1*VV2*U4/DSINH(E1)-DKK*
     &(-BB)**2.*U2*DSINH(E2)*AJ1*VV1*U4/DSINH(E1)-DKK*(-BB)**2.*U3
     &*DCOSH(E2)*PAJ1*VV1*U4/DSINH(E1))*DEXP(DKK)
      AN2(II)=WET(II)*N*(-DKK*CC**2.*RAD(1)*U3*DSINH(E3)*AJ1*U4*VV2/
     &DSINH(E1)+DKK*CC**2.*RAD(1)*U2*DCOSH(E3)*PAJ1*VV2*U4
```

```
     &/DSINH(E1)
     &+DKK*(-BB)**2.*RAD(1)*U3*DSINH(E2)*AJ1*VV1*U4/DSINH(E1)-
     &DKK*(-BB)**2.*RAD(1)*U2*DCOSH(E2)*PAJ1*VV1*U4/DSINH(E1))*
     &DEXP(DKK)
2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN(IJ)
      SM2=SM2+AN1(IJ)
      SM3=SM3+AN2(IJ)
1999  CONTINUE
      RETURN
      END




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C                 FOR LINEAR TEMPERATURE PROFILE                        C
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      SUBROUTINE XRD(N,BB,CC,IN,RAD,U2,U3,U4,U5,DDK,WET,SM1,SM2,SM3)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION WET(96),DDK(96),AN(96),RAD(2),AN1(96),AN2(96)
      DO 2001 II=1,IN
      ZZ=RAD(1)*U2
      XX=RAD(1)*U3*U4
      YY=RAD(1)*U3*U5
      E3=DDK(II)*(ZZ+BB)
      E2=DDK(II)*(ZZ-CC)
      E1=DDK(II)*(BB+CC)
      DK=DDK(II)*RAD(1)*U3
      DKK=DDK(II)
      DK1=RAD(1)*U3
      CALL BESSEL(DK,AJ,AJ0,AJ1,AJ2)
      PAJ1=.5*(AJ0-AJ2)

      CALL BEST(N,1,1,0,DKK,-BB,VV1)
      CALL BEST (N,1,1,0,DKK,CC,VV2)
      AN(II)=WET(II)*(-DKK*(CC)**2.*DSINH(E3)*AJ1*VV2/DSINH(E1)+DKK*
     & (-BB)**2.*AJ1*VV1*DSINH(E2)/DSINH(E1))*DEXP(DKK)

      AN1(II)=WET(II)*(-DKK**2.*CC**2.*U2*DCOSH(E3)*AJ1*U4*VV2/DSINH(
```

```
     & E1)-DKK**2.*CC**2.*U3*DSINH(E3)*PAJ1*VV2*U4/DSINH(E1)+DKK**2.*
     & (-BB)**2.*U2*DCOSH(E2)*AJ1*VV1*U4/DSINH(E1)+DKK**2.*(-BB)**2.*U3
     & *DSINH(E2)*PAJ1*VV1*U4/DSINH(E1))*DEXP(DKK)

      AN2(II)=WET(II)*(DKK**2.*CC**2.*RAD(1)*U3*DCOSH(E3)*AJ1*U4*VV2/
     &DSINH(E1)-DKK**2.*CC**2.*RAD(1)*U2*DSINH(E3)*PAJ1*VV2*U4/DSINH(E1)
     &-DKK**2.*(-BB)**2.*RAD(1)*U3*DCOSH(E2)*AJ1*VV1*U4/DSINH(E1)+
     &DKK**2.*(-BB)**2.*RAD(1)*U2*DSINH(E2)*PAJ1*VV1*U4/DSINH(E1))*
     & DEXP(DKK)

2001  CONTINUE
      SM1=0.D0
      SM2=0.D0
      SM3=0.D0
      DO 1999 IJ=1,IN
      SM1=SM1+AN(IJ)
      SM2=SM2+AN1(IJ)
      SM3=SM3+AN2(IJ)
1999  CONTINUE
      RETURN
      END
```